Retention Indices for Frequently Reported Compounds of Plant Essential Oils

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Gas chromatographic retention indices were evaluated for 505 frequently reported plant essential oil components using a large retention index database. Retention data are presented for three types of commonly used stationary phases: dimethyl silicone (nonpolar), dimethyl silicone with 5% phenyl groups (slightly polar), and polyethylene glycol (polar) stationary phases. The evaluations are based on the treatment of multiple measurements with the number of data records ranging from about 5 to 800 per compound. Data analysis was limited to temperature programmed conditions. The data reported include the average and median values of retention index with standard deviations and confidence intervals. © *2011 by the U.S. Secretary of Commerce on behalf of the United States. All rights reserved.* [doi:10.1063/1.3653552]

Key words: essential oils; gas chromatography; Kováts indices; linear indices; retention indices; identification; flavor; olfaction.

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1. Introduction

The practical applications of plant essential oils are very diverse. They are used for the production of food, drugs, perfumes, aromatherapy, and many other applications.[1–4] The need for identification of essential oil components ranges from product quality control to basic research. The identification of unknown compounds remains a complex problem, in spite of great progress made in analytical techniques over the last several decades.[3,5,6] Gas chromatography (GC) and gas chromatography-mass spectrometry (GC/MS) techniques are commonly employed for the identification of essential oil components.[1,3,7,8] Measurement of retention indices (RI) of chemical compounds and comparison with available retention data collections is the usual approach in the confirmation of compound identification. Retention data are more useful in combination with mass spectrometry, because the combination can provide a nearly unambiguous identification of isomers, which is difficult using mass spectra alone. Thus differences in the structures of branched alkyl substituents and *cis*/*trans* isomers, which normally do not result in significant mass spectral differences, can be identified with the use of retention data.

Gas chromatographic retention data are very attractive for applications due to the simplicity of the measurements, application, and interpretation. To some extent retention data are available at no additional cost or effort as a by-product of the use of chromatographic separation for mass spectrometry measurements. It is known that a large number of components of plant essential oils are common to many species. Adams[7] indicated that the ability to identify 500 compounds would enable one to identify more than 90% of the constituents of an essential oil of most species. Thus a relatively small and reliable RI data collection can substantially increase the identification effectiveness in the analysis of essential oil constituents.

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The purpose of this communication is to evaluate retention indices for the most frequently reported components of essential oils using the retention data from the NIST data-collection.[9–13] A large body of gas chromatographic retention data exists for the compounds of essential oils, thus reliable values of RI data can be provided. The goal was to evaluate retention data for about 500 commonly identified components of essential oils. We undertake the analysis of data distributions of multiple (replicate) measurements to provide statistically justified RI values.

Retention indices also find applications in the characterization of selectivity of stationary phases, in structural analysis, and in studies of physico-chemical properties of analytes and stationary phases.[5,14] Relationships between Kováts indices and thermodynamic properties are used for determination of vapor pressures, enthalpies, and entropies of adsorption and vaporization of different analytes.[15–28] Zabiegala *et al.*[29] employed retention indices for the estimation of the calibration constants of permeation passive samplers with polydimethylsiloxane membranes. RI is also used as an aid in the development of new medical and perfume formulations.[8,30]

The current status of retention data collections and of the development of computerized databases has been summarized by Babushok *et al.*[9] The collection and processing of gas chromatographic properties of chemical compounds began at NIST in the late 1990s with the aim of developing a comprehensive and evaluated database of retention indices.[9,13] Currently the collection contains 346 757 data records for 70 839 compounds measured on nonpolar and polar stationary phases (a data record corresponds to a single RI measurement for chemical compound). Data were extracted from original papers, technical reports, conference proceedings, and Internet sources (1958–2011). The collection contains over 10 000 sources of gas chromatographic properties. The third release of the RI database is available as a part of NIST/EPA/NIH Mass Spectral database (June, 2011),[11] as well as on the Internet (NIST Chemistry WebBook).[12] The database allows one to study and evaluate retention index variability for different chemical compounds. This variability results from the differences in the column properties (brand, column size, etc.), differences in the conditions of measurements, and experimental errors.

2. Retention Indices

The retention index system suggested first by Kováts,[31] and its modification to temperature programming conditions,[5,32] allows the results measured in one laboratory to be used in other laboratories. The retention index combines two fundamental gas chromatographic properties: the relative retention and the specific retention volume.[33] Figuratively speaking, Kováts[31] suggested a chemical ruler to characterize different chemical compounds on a specific time scale for identification purposes. According to Kováts, an analyte's index is its relative time position between the nearest n-alkanes which elute immediately before and after a target analyte. Isothermal Kováts retention indices are determined by the relationship,[31]

$$I_x = 100n + 100[\log(t'_x) - \log(t'_n)]/[\log(t'_{n+1}) - \log(t'_n)], \quad (1)$$

where t'_n and t'_{n+1} are adjusted retention times of the reference n-alkane hydrocarbons eluting immediately before and after compound "X," and t_x is the adjusted retention time of compound "X." Linear indices (nonisothermal indices in accord with the definition of Van den Dool and Kratz[32] from temperature-programming measurements) are defined by the following:

$$I_x = 100n + 100(t_x - t_n)/(t_{n+1} - t_n), \quad (2)$$

where t_n, t_{n+1}, and t_x are net retention times.

A large volume of retention data is available for essential oil compounds. Thus 1967 data records for limonene can be found in the last release of the NIST database. The observed RI data distributions are the result of several factors including small variations in stationary phase polarity, temperature conditions, and ratios between amounts of characterized analytes and reference compounds.[34] The observed data spread is also the result of errors in measurements and compound misidentification.[35] Discussion of retention data distributions can be found in Refs. 9, 10, 35, and 36.

3. Retention Data Presentation and Discussion

A list of the most frequently reported compounds was generated based on the number of data records available for different compounds in the NIST database.[9,11,12] At first, the list of compounds was determined based on the number of all available data records in the database. This list was adjusted in accord with the frequency of data reporting in the journals publishing the results of research related to the essential oils, such as "Journal of Essential Oil Research," "Flavor and Fragrance Journal," "Phytochemistry," and "Biochemical Systematics and Ecology." Additionally, we verified the presence of these compounds in the available collections of data for essential oil compounds.[6,7,37–39] As the result, the list of frequently reported components of essential oils was determined (Table 1). We limited our analysis to the 505 commonly identified compounds. Only compounds with at least five data-records were included in the final list.

The following describes our procedure for the treatment of the retention data for these compounds. The data treatment was limited to the three commonly used nonpolar and polar stationary phases: dimethylsilicone stationary phase (OV-101, HP-1, DB-1, SE-30, etc.), dimethylsilicone phase with 5% phenyl groups (DB-5, SE-54, HP-5, Ultra-2, etc.), and polyethylene glycol stationary phase (polar phase, e.g., Carbowax 20M, Innowax, CP-Wax 52 CB). Another constraint was the use of RI data measured under temperature programmed conditions. In this work, we used an approach[35,36] to RI data distribution analysis to extract the values of retention indices, corresponding to the conditions typically used for gas chromatographic measurements.

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Prior to calculation of the data distribution characteristics, outlier RI values were deleted based on the data review. Data points separated by more than 10 iu (index units) from the main group of data, were not considered. Exceptions were cases with a small number of data records and compounds with large spans of retention values. For such cases data records were analyzed and decisions were made taking into account several factors such as the origin of the data, data consistency with other measurements, measurement conditions, procedure of identification, procedure of index determination, etc. Overall not more than 5% of data points were deleted as outliers.

The preparation of the NIST retention database (2005, 2008, and 2011 releases) included a data review aimed at eliminating erroneous data. This data screening was mainly concentrated on the correct naming, structure presentation, data entry corrections, verification of experimental conditions, and consistency with retention data for other compounds including the elution order.[9,11,12] The data review additionally included a comparison of database RI values with the predicted retention indices using the procedure suggested by Stein *et al.*,[10] and included the analysis of retention index distributions for compounds, where large data spans were found. As a result data found to be in error were deleted, and suspicious RI values were flagged. Thus, to some extent, the analyzed retention data were already selected as "reasonably sound" experimental RI values.

For each compound, the following values were determined: average and median values of retention indices, standard deviation, and confidence intervals (50% and 90% of RI data ranges). If the dataset of available measurements was less than 20 data-records, a range of retention indices was provided instead. Of course, the distributions of analyzed RI data do not represent strictly random data. The observed deviations from the average value are a combination of random and systematic errors, where the systematic deviations represent significant contributions. Where there was a problem with treatment of retention data (e.g., for distributions with two groups of data or with a large span of retention values), the range of available RI measurements was provided. In this work, all considered RI data-records were treated as equivalent data.

Tables 2–4 contain the results of the determination of RI values for the most frequently reported components of essential oils. The following data are presented for each compound (Tables 1–5):

– name of the compound,
– CAS registry number,
– molecular formula,
– number of replicate measurements for compound,
– median value,
– average value,
– standard deviation,
– confidence intervals (50% and 90% range of RI data values),
– comment.

Data are ordered in accord with the RI value (average value). Additionally, the cross-reference Table 1 contains the data ordered alphabetically by compound name. For compound naming, we employed mainly the commonly used names of constituents of essential oils. Most of these names correspond those used in publications.[7,37,38,66] Additional descriptors (prefixes), such as *cis*-, *trans*-, *exo*-, *endo*-, *epi*, etc., are placed after the key chemical name. Table 1 contains also systematic names of components along with the CAS registry numbers and molecular formula. Other names (systematic names, synonyms, trade names), structures, and the original RI data with references can be found in the NIST/EPA/NIH MS database[11] and the NIST Chemistry WebBook.[12]

There were a number of cases with different assignments of CAS registry numbers supposedly to the same compound. These differences mostly have two causes (not considering erroneously assigned CAS registry numbers). One common cause is the use of different conventions for compound naming. Thus, RI data for the same isomer of sabinene hydrate can be found labeled as *cis*- or *trans*-depending on the convention used. This naturally leads to some confusion in the data treatment. Second is the use of registry numbers corresponding to different enantiomers, or to the racemic mixture, or the use of the CAS number for an unknown isomer. Thus the same compound can sometimes be found under different CAS registry numbers. The retention characteristics of enantiomers are practically indistinguishable on the stationary phases considered in this article, and sometimes authors were not able to provide accurate identification using only GC-MS measurements (separation of enantiomers requires application of specially designed chiral stationary phases). For compounds where different registry numbers can be found in literature, we provided several registry numbers with the corresponding names (Table 2).

An important gas-chromatographic characteristic of organic compounds is their elution order. It is a highly reproducible characteristic, and it is often used for the identification of isomers in mixtures. It is commonly regarded that for a given type of stationary phase, the elution order of compounds is a more accurate piece of retention data than the retention indices. For most of the compounds considered, the evaluated RI values are consistent with data[7] on the elution order (dimethylsilicone with 5% phenyl groups). The observed inconsistencies (in comparison with the data of Adams[7]) are within the calculated error ranges. We did not analyze the available data for the elution order of essential oil components. We believe that much more work is required for the proper evaluation of elution order data. It is also of interest to consider optimization of retention index values through the analysis of available elution order data.

A large number of retention data sources were involved in the data evaluation (more than 3000). The work is based on the analysis of a very large set of data. We do not feel that this article is the place to provide all of the references for the retention data analyzed. The references of data sources are provided as the electronic supplementary material.[98] These

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can also be found in NIST/EPA/NIH-MS-database[11] and the NIST Chemistry WebBook.[12]

Table 6 gives the average standard deviations and averaged confidence intervals for the components of essential oils listed in Tables 3–5 for three stationary phases. The averaged standard deviations are in the following order in accord with the phase used: polyethylene glycol > dimethylsilicone > dimethylsilicone with 5% phenyl groups. It is of interest that the obtained average confidence intervals are relatively narrow. Thus, approximately 50% of RI measurements could be found in the 6.7 iu range for typical constituents of essential oils, and 90% of measurements belong to 25.5 iu range for identifications made on dimethylsilicone phase with 5% phenyl groups. The calculated average standard deviations and confidence intervals can be considered as reasonable estimates for characterization of the RI variability of the common constituents of essential oils. These estimates can be used in automated identification procedures as constraints for removing false-positive identifications (RI search windows).

A great advantage of chromatographic techniques is the ability to distinguish different diastereomers. The diastereomers are characterized by practically identical mass spectra, and the use of GC retention parameters is often the only practical method for the correct identification of such isomers. Unfortunately there are currently no theoretical methods for prediction of retention behavior of such diastereomers. The difficulties of identification can be seen for four (Z,E)-isomers of farnesol (3,7,11-trimethyldodeca-2,6,10-trien-1-ol). Table 7 contains a comparison of estimated retention data using the NIST database with the data listed in the two editions of Adams' book[7,53] for the same isomers on nonpolar and slightly polar phases. As can be seen, the relative elution order of isomers obtained corresponds well to the elution order provided in the 2003 edition.[53] However, the 2007 edition[7] contains retention data significantly different from these estimates. Thus, the identification of farnesol isomers can formally be uncertain. In any case, authors should indicate the source of chromatographic information used for isomer assignments. Additionally, Table 7 includes the results of identification of farnesol isomers (elution order) made with the use of other analytical techniques and comparisons with authentic samples.[92–97] Based on these data, we re-considered the results of our estimates and re-assigned the obtained retention indices in accord with the elution order of isomers observed in Refs. 92–97 (Table 4), which is consistent with data.[7]

Literature data show that RI values for low-polarity polar stationary phases (like dimethylsilicone phase with 5% phenyl groups) are usually slightly higher than the RI values for nonpolar phases (dimethylsilicone). The differences are within 5 iu to 30 iu depending on the polarity of analytes. However, it was observed that for several compounds the retention indices were approximately the same for both phases and sometimes larger RI values were observed for the dimethylsilicone phase. These compounds are marked in Table 1. In general, the differences in RI values do not exceed the sum of their standard deviations for these stationary phases. These anomalies are possibly the result of measurement inaccuracies. Another cause of such behavior might be the influence of the polarity of analytes with the active hydrogen atoms in hydroxyl groups. Slight asymmetry of GC peaks on nonpolar phases with the shift of the maximums of the chromatographic peaks is observed for such compounds. The use of slightly polar stationary phases decreases the asymmetry of the peaks of polar compounds and their tailing.

TABLE 1. Cross-reference list of essential oil components (common names, other chemical identifiers and average retention index values)[a,b]

Name	Systematic name	CAS	Formula	RI(DIMS)	RI(DIMS5P)	RI(PEG)
Abietadiene	Phenanthrene, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,1,4a-trimethyl-7-(1-methylethyl)-, [4aS-(4aα,4bβ,10aβ)]-	35241-40-8	$C_{20}H_{32}$	2061.8	2080.5	[2450]
Abietatriene	Phenanthrene, 1,2,3,4,4a,9,10,10a-octahydro-1,1,4a-trimethyl-7-(1-methylethyl)-, (4aS-trans)-	19407-28-4	$C_{20}H_{30}$	2032.8	2054.3	2506.1
Acetic acid		64-19-7	$C_2H_4O_2$	633.0	622.3	1446.1
Acetoin	2-Butanone, 3-hydroxy-	513-86-0	$C_4H_8O_2$	684.3	713.7	1282.2
Acetophenone	1-Phenylethanone	98-86-2	C_8H_8O	1041.5	1067.4	1647.6
2-Acetylfuran		1192-62-7	$C_6H_6O_2$	883.8	912.4	1498.8
β-Acoradiene	Spiro[4.5]dec-7-ene, 1,8-dimethyl-4-(1-methylethenyl)-, [1R-(1α,4β,5α)]-	28477-64-7	$C_{15}H_{24}$	1461.8	1465.5	1687.7
α-Acorenol	Spiro[4.5]dec-7-ene-1-methanol, α,α,4,8-tetramethyl-, [1R-(1α,4β,5α)]-	28296-85-7	$C_{15}H_{26}O$	1620.3	1630.0	[2163]
Alloaromadendrene	1H-Cycloprop[e]azulene, decahydro-1,1,7-trimethyl-4-methylene-, [1aR-(1aα,4aβ,7α,7aβ,7bα)]-	25246-27-9	$C_{15}H_{24}$	1459.1	1459.9	1649.2
allo-Ocimene	2,4,6-Octatriene, 2,6-dimethyl-, (E,Z)-	7216-56-0	$C_{10}H_{16}$	1116.4	1129.9	1366.5
α-Amorphene	1β,7βH-Cadina-4,9-diene	20085-19-2	$C_{15}H_{24}$	1466.2	1482.4	1693.1
Anethole, (E)-	Benzene, 1-methoxy-4-(1-propenyl)-, (E)-	4180-23-8	$C_{10}H_{12}O$	1264.7	1285.2	1826.1
p-Anisaldehyde	Benzaldehyde, 4-methoxy-	123-11-5	$C_8H_8O_2$	1222.7	1251.8	2010.7
p-Anisyl alcohol	Benzyl alcohol, p-methoxy-	105-13-5	$C_8H_{10}O_2$	1249.7	1282.3	[2268]

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TABLE 1. Cross-reference list of essential oil components (common names, other chemical identifiers and average retention index values)[a,b]—Continued

Name	Systematic name	CAS	Formula	RI(DIMS)	RI(DIMS5P)	RI(PEG)
Ar-Curcumene	Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-	644-30-4	$C_{15}H_{22}$	1471.4	1482.2	1773.5
Aromadendrene	1H-Cycloprop[e]azulene, decahydro-1,1,7-trimethyl-4-methylene-, [1aR-(1aα,4aα,7α,7aβ,7bα)]-	489-39-4	$C_{15}H_{24}$	1439.0	1440.6	1620.2
Artemisia alcohol	1,5-Heptadien-4-ol, 3,3,6-trimethyl-	27644-04-8	$C_{10}H_{18}O$	1071.5	1083.1	[1510]
Artemisia ketone	1,5-Heptadien-4-one, 3,3,6-trimethyl-	546-49-6	$C_{10}H_{16}O$	1048.3	1062.0	1344.7
Benzaldehyde	Phenylformaldehyde	100-52-7	C_7H_6O	936.6	962.7	1518.7
Benzeneacetaldehyde	Phenylacetaldehyde	122-78-1	C_8H_8O	1016.1	1045.9	1640.7
Benzyl acetate	Acetic acid, benzyl ester	140-11-4	$C_9H_{10}O_2$	1141.1	1165.6	1723.1
Benzyl alcohol	Phenylmethanol	100-51-6	C_7H_8O	1015.4	1036.9	1865.3
Benzyl benzoate	Benzoic acid, phenylmethyl ester	120-51-4	$C_{14}H_{12}O_2$	1733.5	1761.3	2612.7
Benzyl salicylate	Benzoic acid, 2-hydroxy-, phenylmethyl ester	118-58-1	$C_{14}H_{12}O_3$	1837.2	1867.4	2787.5
α-Bergamotene, cis-	Bicyclo[3.1.1]hept-2-ene, 2,6-dimethyl-6-(4-methyl-3-pentenyl)-, (1α,5α,6β)-	18252-46-5	$C_{15}H_{24}$	1410.3	1414.5	1559.1
α-Bergamotene, trans-	Bicyclo[3.1.1]hept-2-ene, 2,6-dimethyl-6-(4-methyl-3-pentenyl)-, [1S-(1α,5α,6α)]-	13474-59-4	$C_{15}H_{24}$	1431.1	1434.5	1575.7
Bicycloelemene	Bicyclo[4.1.0]heptane, 3-ethenyl-3,7,7-trimethyl-2-(1-methylethenyl)-, [1R-(1α,2α,3β,6α)]-	32531-56-9	$C_{15}H_{24}$	1336.2	1333.3	1487.5
Bicyclogermacrene	Bicyclo[8.1.0]undeca-2,6-diene, 3,7,11,11-tetramethyl-, (E,E)-(1S,10R)-(+)-	24703-35-3	$C_{15}H_{24}$	1489.8	1494.1	1734.5
β-Bisabolene	1,5-Heptadiene, 6-methyl-2-(4-methyl-3-cyclohexen-1-yl)-, (S)-(-)-	495-61-4	$C_{15}H_{24}$	1499.9	1508.4	1727.5
α-Bisabolene, (E)-	2,5-Heptadiene, 2-methyl-6-(4-methyl-3-cyclohexen-1-yl)-, (E)-	25532-79-0	$C_{15}H_{24}$	1533.6	1540.3	1775.2
γ-Bisabolene, (E)-	Cyclohexene, 4-(1,5-dimethyl-4-hexenylidene)-1-methyl-, (E)-	53585-13-0	$C_{15}H_{24}$	1525.6	1532.9	1744.7
α-Bisabolene, (Z)-	2,5-Heptadiene, 2-methyl-6-(4-methyl-3-cyclohexen-1-yl)-, (Z)-	29837-07-8	$C_{15}H_{24}$	1496.2	1503.1	1740.4
γ-Bisabolene, (Z)-	Cyclohexene, 4-(1,5-dimethyl-4-hexenylidene)-1-methyl-, (Z)-	13062-00-5	$C_{15}H_{24}$	1511.7	1511.6	1750.5
α-Bisabolol[c]	3-Cyclohexene-1-methanol, α,4-dimethyl-α-(4-methyl-3-pentenyl)-, (αR,1R)-rel-	515-69-5	$C_{15}H_{26}O$	1668.4	1682.8	2213.6
β-Bisabolol	3-Cyclohexen-1-ol, 1-[(1S)-1,5-dimethyl-4-hexenyl]-4-methyl-, (1S)-	15352-77-9	$C_{15}H_{26}O$	1658.6	1672.0	2143.1
α-Bisabolol, epi-[c]	3-Cyclohexene-1-methanol, α,4-dimethyl-α-(4-methyl-3-pentenyl)-, (αR,1R)-	23178-88-3	$C_{15}H_{26}O$	1674.3	1685.3	2214.3
Borneol[c]	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, endo-	507-70-0	$C_{10}H_{18}O$	1153.2	1166.2	1699.6
Bornyl acetate	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, acetate, endo-	76-49-3	$C_{12}H_{20}O_2$	1270.2	1283.5	1579.3
Bornyl formate	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, formate, endo-	7492-41-3	$C_{11}H_{18}O_2$	[1208]	1222.6	1595.1
β-Bourbonene	Cyclobuta[1,2:3,4]dicyclopentene, decahydro-3a-methyl-6-methylene-1-(1-methylethyl)-, [1S-(1α,3aα,3bβ,6aβ,6bα)]-	5208-59-3	$C_{15}H_{24}$	1381.7	1384.2	1523.2
α-Bulnesene	Azulene, 1,2,3,5,6,7,8,8a-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1S-(1α,7α,8aβ)]-	3691-11-0	$C_{15}H_{24}$	1500.6	1504.1	[1629]
Bulnesol	5-Azulenemethanol, 1,2,3,3a,4,5,6,7-octahydro-α,α,3,8-tetramethyl-, [3S-(3α,3aβ,5α)]-	22451-73-6	$C_{15}H_{26}O$	1653.3	1665.7	2205.3
Butan-1-ol, 2-methyl-		137-32-6	$C_5H_{12}O$	721.9	740.8	1205.8
Butanal, 2-methyl-		96-17-3	$C_5H_{10}O$	642.8	660.2	915.5
2,3-Butanedione		431-03-8	$C_4H_6O_2$	565.6	596.6	977.6
Butanoic acid		107-92-6	$C_4H_8O_2$	806.8	808.3	1623.7
Butanoic acid, 2-methyl-		116-53-0	$C_5H_{10}O_2$	828.2	861.9	1664.5
1-Butanol		71-36-3	$C_4H_{10}O$	651.6	660.2	1139.6
2-Buten-1-ol, 3-methyl-		556-82-1	$C_5H_{10}O$	750.6	774.6	1316.1
Cadalene	Naphthalene, 4-isopropyl-1,6-dimethyl-	483-78-3	$C_{15}H_{18}$	1654.9	1671.3	[2233]
Cadina-1(2),4-diene, cis	Naphthalene, 1,2,3,4,4a,7-hexahydro-1,6-dimethyl-4-(1-methylethyl)-, [1S-(1α,4α,4aα)]-	29837-12-5	$C_{15}H_{24}$	1523.9	1531.0	1788.0
α-Cadinene[c]	Naphthalene, 1,2,4a,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1α,4aβ,8aα)-	82468-90-4	$C_{15}H_{24}$	1526.6	1533.3	1769.1
γ-Cadinene	Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-7-methyl-4-	39029-41-9	$C_{15}H_{24}$	1505.7	1513.1	1763.3

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TABLE 1. Cross-reference list of essential oil components (common names, other chemical identifiers and average retention index values)[a,b]—Continued

Name	Systematic name	CAS	Formula	RI(DIMS)	RI(DIMS5P)	RI(PEG)
	methylene-1-(1-methylethyl)-, (1α,4aβ,8aα)-					
δ-Cadinene	Naphthalene, 1,2,3,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1S-cis)-	483-76-1	$C_{15}H_{24}$	1513.9	1523.2	1755.7
α-Cadinol	1-Naphthalenol, 1,2,3,4,4a,7,8,8a-octahydro-1,6-dimethyl-4-(1-methylethyl)-, [1R-(1α,4β,4aβ,8aα)]-	481-34-5	$C_{15}H_{26}O$	1640.2	1651.9	2227.3
α-Cadinol, epi-	1-Naphthalenol, 1,2,3,4,4a,7,8,8a-octahydro-1,6-dimethyl-4-(1-methylethyl)-, [1S-(1α,4α,4aα,8aβ)]-	5937-11-1	$C_{15}H_{26}O$	1626.4	1637.8	2169.7
α-Calacorene	Naphthalene, 1,2-dihydro-4,7-dimethyl-1-(1-methylethyl)-, (S)-	21391-99-1	$C_{15}H_{20}$	1530.4	1540.3	1921.4
β-Calacorene	Naphthalene, 1,2,3,4-tetrahydro-6-methyl-1-methylene-4-(1-methylethyl)-	50277-34-4	$C_{15}H_{20}$	1547.1	1559.4	1940.3
Calamenene, cis-[c]	Naphthalene, 1,2,3,4-tetrahydro-1,6-dimethyl-4-(1-methylethyl)-, cis-	72937-55-4	$C_{15}H_{22}$	1509.6	1522.9	1834.5
Calamenene, trans-	Naphthalene, 1,2,3,4-tetrahydro-1,6-dimethyl-4-(1-methylethyl)-, trans-	73209-42-4	$C_{15}H_{22}$	1512.8	1528.3	1823.0
Camphene[c]	2,2-Dimethyl-3-methylenebicyclo[2.2.1]heptane	79-92-5	$C_{10}H_{16}$	947.4	950.3	1068.5
Camphene hydrate	Bicyclo[2.2.1]heptan-2-ol, 2,3,3-trimethyl-	465-31-6	$C_{10}H_{18}O$	1135.8	1148.7	[1602]
α-Campholenal	3-Cyclopentene-1-acetaldehyde, 2,2,3-trimethyl-, (R)-	4501-58-0	$C_{10}H_{16}O$	1106.8	1124.1	1496.0
Camphor[c]	1,7,7-Trimethylbicyclo[2.2.1]-2-heptanone	76-22-2	$C_{10}H_{16}O$	1125.0	1143.4	1515.1
3-Carene	Bicyclo[4.1.0]hept-3-ene, 3,7,7-trimethyl-	13466-78-9	$C_{10}H_{16}$	1007.2	1011.3	1146.8
δ-2-Carene	Bicyclo[4.1.0]hept-2-ene, 3,7,7-trimethyl-	554-61-0	$C_{10}H_{16}$	997.7	1003.3	1133.9
Carotol	3a(1H)-Azulenol, 2,3,4,5,8,8a-hexahydro-6,8a-dimethyl-3-(1-methylethyl)-, [3R-(3α,3aα,8aα)]-	465-28-1	$C_{15}H_{26}O$	1592.8	1595.3	2027.6
Carvacrol	2-Methyl-5-(1-methylethyl)phenol	499-75-2	$C_{10}H_{14}O$	1282.7	1300.4	2210.8
Carvacrol acetate	Phenol, 2-methyl-5-(1-methylethyl)-, acetate	6380-28-5	$C_{12}H_{16}O_2$	1354.4	1373.1	1880.1
Carvacrol, methyl ether	Benzene, 2-methoxy-1-methyl-4-(1-methylethyl)-	6379-73-3	$C_{11}H_{16}O$	1221.5	1243.0	1598.9
Carveol, cis-	2-Cyclohexen-1-ol, 2-methyl-5-(1-methylethenyl)-, cis-	1197-06-4	$C_{10}H_{16}O$	1206.4	1226.7	1854.4
Carveol, trans-	2-Cyclohexen-1-ol, 2-methyl-5-(1-methylethenyl)-, trans-	1197-07-5	$C_{10}H_{16}O$	1200.9	1217.1	1836.3
Carvone[c]	2-Methyl-5-(1-methylethenyl)-2-cyclohexen-1-one	99-49-0	$C_{10}H_{14}O$	1218.0	1242.0	1733.6
Carvotanacetone	2-Cyclohexen-1-one, 2-methyl-5-(1-methylethyl)-, (S)-	499-71-8	$C_{10}H_{16}O$	1221.0	1245.3	1687.7
Carvyl acetate, cis-	2-Cyclohexen-1-ol, 2-methyl-5-(1-methylethenyl)-, acetate, cis-	1205-42-1	$C_{12}H_{18}O_2$	1334.4	1362.0	[1775]
Carvyl acetate, trans-	2-Cyclohexen-1-ol, 2-methyl-5-(1-methylethenyl)-, acetate, trans-	1134-95-8	$C_{12}H_{18}O_2$	1321.9	1336.6	[1727]
Caryophylla-4(12),8(13)-dien-5α-ol	Bicyclo[7.2.0]undecan-5-ol, 10,10-dimethyl-2,6-dimethylene-, (1S,5R,9R)-(+)-	19431-79-9	$C_{15}H_{24}O$	1623.9	1640.3	2301.0
Caryophyllene oxide	5-Oxatricyclo[8.2.0.04,6]dodecane, 4,12,12-trimethyl-9-methylene-, (1R,4R,6R,10S)-	1139-30-6	$C_{15}H_{24}O$	1570.0	1580.6	1986.2
Caryophyllene, (E)-	Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, (E)-(1R,9S)-(-)-	87-44-5	$C_{15}H_{24}$	1419.3	1420.1	1598.5
Caryophyllene, (Z)-	Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, (Z)-(1R,9S)-(-)-	118-65-0	$C_{15}H_{24}$	1407.7	1406.5	1588.2
Caryophyllenol II	Bicyclo[7.2.0]undec-3-en-5-ol, 4,11,11-trimethyl-8-methylene-, (1R,3E,5R,9S)-	32214-89-4	$C_{15}H_{24}O$	[1655]	1659.7	[2392]
Caryophyllenyl alcohol		-	$C_{15}H_{26}O$	1560.0	1568.6	[2044]
α-Cedrene	1H-3a,7-Methanoazulene, 2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-, [3R-(3α,3aβ,7β,8aα)]-	469-61-4	$C_{15}H_{24}$	1410.9	1412.2	1582.9
β-Cedrene	1H-3a,7-Methanoazulene, octahydro-3,8,8-trimethyl-6-methylene-, [3R-(3α,3aβ,7β,8aα)]-	546-28-1	$C_{15}H_{24}$	1417.7	1422.4	1611.1
Cedrol	1H-3a,7-Methanoazulen-6-ol, octahydro-3,6,8,8-tetramethyl-, [3R-(3α,3aβ,6α,7β,8aα)]-	77-53-2	$C_{15}H_{26}O$	1597.1	1600.1	2119.6
Chamazulene	1,4-Dimethyl-7-ethylazulene	529-05-5	$C_{14}H_{16}$	1710.0	1726.7	[2430]
β-Chamigrene	(-)-3,7,7-Trimethyl-11-methylenespiro[5.5]undec-2-ene	18431-82-8	$C_{15}H_{24}$	1470.1	1478.9	1723.9
Chavicol	Phenol, 4-(2-propenyl)-	501-92-8	$C_9H_{10}O$	1236.9	1253.9	2337.0
Chrysanthenol, cis-	Bicyclo[3.1.1]hept-2-en-6-ol, 2,7,7-trimethyl-, (1α,5α,6α)-	55722-60-6	$C_{10}H_{16}O$	1150.3	1162.9	1762.0
Chrysanthenone	Bicyclo[3.1.1]hept-2-en-6-one, 2,7,7-trimethyl-	473-06-3	$C_{10}H_{14}O$	1104.3	1124.5	1507.6
Chrysanthenyl acetate, cis-	Bicyclo[3.1.1]hept-2-en-6-ol, 2,7,7-trimethyl-, acetate, (1α,5α,6α)-	67999-48-8	$C_{12}H_{18}O_2$	1248.4	1261.8	1561.1

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TABLE 1. Cross-reference list of essential oil components (common names, other chemical identifiers and average retention index values)[a,b]—Continued

Name	Systematic name	CAS	Formula	RI(DIMS)	RI(DIMS5P)	RI(PEG)
1,4-Cineole	7-Oxabicyclo[2.2.1]heptane, 1-isopropyl-4-methyl-	470-67-7	$C_{10}H_{18}O$	1008.9	1016.8	1186.3
1,8-Cineole	2-Oxabicyclo[2.2.2]octane, 1,3,3-trimethyl-	470-82-6	$C_{10}H_{18}O$	1022.4	1031.8	1211.1
Cinnamaldehyde, cis-	2-Propenal, 3-phenyl-, (Z)-	57194-69-1	C_9H_8O	1178.0	1215.2	[1879]
Cinnamaldehyde, trans-	2-Propenal, 3-phenyl-, (E)-	14371-10-9	C_9H_8O	1238.6	1271.3	2033.2
Citronellal	3,7-Dimethyl-6-octenal	106-23-0	$C_{10}H_{18}O$	1133.6	1153.7	1475.3
Citronellol	3,7-Dimethyl-6-octen-1-ol	106-22-9	$C_{10}H_{20}O$	1212.4	1228.1	1763.9
Citronellyl acetate	3,7-Dimethyl-6-octen-1-yl acetate	150-84-5	$C_{12}H_{22}O_2$	1335.6	1352.4	1656.5
Citronellyl butanoate	3,7-Dimethyl-6-octenyl butanoate	141-16-2	$C_{14}H_{26}O_2$	1506.2	1528.6	[1765]
Citronellyl formate	3,7-Dimethyl-6-octen-1-ol formate	105-85-1	$C_{11}H_{20}O_2$	1260.4	1276.7	1615.2
β-Copaen-4α-ol	Tricyclo[4.4.0.02,7]decan-4-ol, 1-methyl-3-methylene-8-(1-methylethyl)-, (1R,2R,4S,6S,7S,8S)-rel-	124753-76-0	$C_{15}H_{24}O$	1577.9	1580.2	[2141]
α-Copaene	(1R,2S,6S,7S,8S)-(-)-8-Isopropyl-1,3-dimethyltricyclo[4.4.0.02,7]dec-3-ene	3856-25-5	$C_{15}H_{24}$	1375.5	1376.2	1491.0
β-Copaene	Tricyclo[4.4.0.02,7]decane, 1-methyl-3-methylene-8-(1-methylethyl)-, (1R,2S,6S,7S,8S)-rel-	18252-44-3	$C_{15}H_{24}$	1427.3	1433.1	1579.8
p-Cresol	p-Methylhydroxybenzene	106-44-5	C_7H_8O	1051.7	1077.4	2073.0
p-Cresol, 2-methoxy-	2-Methoxy-4-methylphenol	93-51-6	$C_8H_{10}O_2$	1163.4	1192.9	1954.2
Cryptone	2-Cyclohexen-1-one, 4-isopropyl-	500-02-7	$C_9H_{14}O$	1156.7	1183.6	1674.8
α-Cubebene	1H-Cyclopenta[1,3]cyclopropa[1,2] benzene, 3aα,3bα,4,5,6,7-hexahydro- 4α-isopropyl-3,7β-dimethyl-, (-)-	17699-14-8	$C_{15}H_{24}$	1352.2	1351.4	1460.4
β-Cubebene	1H-Cyclopenta[1,3]cyclopropa[1,2] benzene, octahydro-7-methyl-3-methylene-4-(1-methylethyl)-, (3aS,3bR,4S,7R,7aR)-	13744-15-5	$C_{15}H_{24}$	1383.5	1386.6	1541.7
Cubebol	1H-Cyclopenta[1,3]cyclopropa[1,2] benzen-3-ol, 2,3,3aα,3bα,4,5,6,7-octahydro-4α-isopropyl-3β,7β-dimethyl-, (-)-	23445-02-5	$C_{15}H_{26}O$	1504.9	1514.9	1941.7
Cubebol, epi-	1H-Cyclopenta[1,3]cyclopropa[1,2] benzen-3-ol, octahydro-3,7-dimethyl-4-(1-methylethyl)-, (3R,3aR,3bR,4S,7R,7aR)-	38230-60-3	$C_{15}H_{26}O$	1489.0	1488.9	[1900]
Cubenol	4a(2H)-Naphthalenol, 1,3,4,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, [1S-(1α,4β,4aβ,8aα)]-	21284-22-0	$C_{15}H_{26}O$	1619.9	1636.5	2067.8
Cubenol, 1,10-di-epi-	4a(2H)-Naphthalenol, 1,3,4,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, [1S-(1α,4aα,8aα)]-	73365-77-2	$C_{15}H_{26}O$	1605.5	1612.3	[2074]
1-Cubenol, epi-	4a(2H)-Naphthalenol, 1,3,4,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, [1S-(1α,4β,4aα,8aα)]-	19912-67-5	$C_{15}H_{26}O$	1614.0	1625.5	2088
Cumin aldehyde	Benzaldehyde, p-isopropyl-	122-03-2	$C_{10}H_{12}O$	1212.6	1237.9	1784.1
Cuparene[c]	Benzene, 1-methyl-4-(1,2,2-trimethylcyclopentyl)-, (R)-	16982-00-6	$C_{15}H_{22}$	1504.8	1506.6	1816.1
β-Curcumene	1,4-Cyclohexadiene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-, (R)-	28976-67-2	$C_{15}H_{24}$	1503.0	1512.9	1737.0
γ-Curcumene	1,3-Cyclohexadiene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-, (R)-	28976-68-3	$C_{15}H_{24}$	1472.7	1480.3	1692.1
β-Cyclocitral	1-Formyl-2,6,6-trimethyl-1-cyclohexene	432-25-7	$C_{10}H_{16}O$	1196.1	1218.3	1610.3
Cyclosativene	1,2α,4-Methenoindan, 3aβ,4β,5,6,7,7a-hexahydro-5α-isopropyl-1β,7aβ-dimethyl-	22469-52-9	$C_{15}H_{24}$	1368.4	1368.2	1483.2
p-Cymen-7-ol	4-Isopropylbenzenemethanol	536-60-7	$C_{10}H_{14}O$	1270.1	1287.7	2100.7
p-Cymen-8-ol	1-Methyl-4-(1-hydroxy-1-methylethyl)benzene	1197-01-9	$C_{10}H_{14}O$	1164.6	1183.9	1848.3
m-Cymene	1-Isopropyl-3-methylbenzene	535-77-3	$C_{10}H_{14}$	[1012]	1022.0	1277.0
o-Cymene	1-Isopropyl-2-methylbenzene	527-84-4	$C_{10}H_{14}$	[1032]	1041.0	[1310]
p-Cymene	1-Isopropyl-4-methylbenzene	99-87-6	$C_{10}H_{14}$	1015.1	1024.3	1270.1
p-Cymenene	1-Isopropenyl-4-methylbenzene	1195-32-0	$C_{10}H_{12}$	1073.7	1087.9	1437.5
Cyperene	3H-3a,7-Methanoazulene, 2,4,5,6,7,8-hexahydro-1,4,9,9-tetramethyl-, [3aR-(3aα,4β,7α)]-;	2387-78-2	$C_{15}H_{24}$	1398.7	1397.8	1528.0
β-Damascenone, (E)-	2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (E)-	23726-93-4	$C_{13}H_{18}O$	1363.4	1385.5	1820.9
Daucene	Azulene, 1,2,4,5,8,8a-hexahydro-3-isopropyl-6,8a-dimethyl-	16661-00-0	$C_{15}H_{24}$	1376.8	1380.6	1495.2
2,4-Decadienal, (2E,4E)-		25152-84-5	$C_{10}H_{16}O$	1290.5	1317.6	1808.2
2,4-Decadienal, (2E,4Z)-		25152-83-4	$C_{10}H_{16}O$	1273.1	1296.3	1756.1

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TABLE 1. Cross-reference list of essential oil components (common names, other chemical identifiers and average retention index values)[a,b]—Continued

Name	Systematic name	CAS	Formula	RI(DIMS)	RI(DIMS5P)	RI(PEG)
γ-Decalactone	2(3H)-Furanone, 5-hexyldihydro-	706-14-9	$C_{10}H_{18}O_2$	1426.9	1470.6	2135.3
δ-Decalactone	2H-Pyran-2-one, tetrahydro-6-pentyl-	705-86-2	$C_{10}H_{18}O_2$	1448.0	1498.0	2187.8
Decanal		112-31-2	$C_{10}H_{20}O$	1185.7	1205.4	1495.9
Decanoic acid		334-48-5	$C_{10}H_{20}O_2$	1363.5	1375.5	2273.7
1-Decanol	1-Hydroxydecane	112-30-1	$C_{10}H_{22}O$	1258.5	1272.1	1754.7
2-Decenal, (E)-		3913-81-3	$C_{10}H_{18}O$	1239.1	1263.4	1639.7
Decyl acetate	Acetic acid, decyl ester	112-17-4	$C_{12}H_{24}O_2$	1392.3	1407.1	1677.3
Dehydro-1,8-cineole	2-Oxabicyclo[2.2.2]oct-5-ene, 1,3,3-trimethyl-	66113-06-2	$C_{10}H_{16}O$	979.8	989.8	1192.5
Dendrolasin	Furan, 3-(4,8-dimethyl-3,7-nonadienyl)-, (E)-	23262-34-2	$C_{15}H_{22}O$	1561.3	1576.5	[1954]
Dihydrocarveol	Cyclohexanol, 2-methyl-5-(1-methylethenyl)-, (1α,2β,5α)-	38049-26-2	$C_{10}H_{18}O$	1181.9	1194.5	1707.3
Dihydrocarvone, trans-	Cyclohexanone, 2-methyl-5-(1-methylethenyl)-, trans-	5948-04-9	$C_{10}H_{16}O$	1184.9	1201.4	1623.1
Dill apiole	1,3-Benzodioxole, 4,5-dimethoxy-6-(2-propenyl)-	484-31-1	$C_{12}H_{14}O_4$	1596.3	1621.7	2346.3
1,4-Dimethoxybenzene		150-78-7	$C_8H_{10}O_2$	1138.4	1167.6	[1728]
2,5-Dimethoxy-p-cymene	Benzene, 1,4-dimethoxy-2-methyl-5-(1-methylethyl)-	14753-08-3	$C_{12}H_{18}O_2$	[1407]	1421.4	1868.1
Dimethyl trisulfide	2,3,4-Trithiapentane	3658-80-8	$C_2H_6S_3$	948.3	971.7	1376.2
Dodecanal	Lauraldehyde	112-54-9	$C_{12}H_{24}O$	1389.2	1408.1	1711.5
Dodecanoic acid	Lauric acid	143-07-7	$C_{12}H_{24}O_2$	1563.7	1569.2	2486.5
1-Dodecanol	Lauryl alcohol	112-53-8	$C_{12}H_{26}O$	1459.8	1472.8	1959.3
2-Dodecenal, (E)-		20407-84-5	$C_{12}H_{22}O$	1444.3	1468.4	1865.8
β-Elemene	Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-, [1S-(1α,2β,4β)]-	515-13-9	$C_{15}H_{24}$	1388.0	1390.4	1590.9
γ-Elemene[c]	Cyclohexane, 1-ethenyl-1-methyl-2-(1-methylethenyl)-4-(1-methylethylidene)-, (1R-trans)-	29873-99-2	$C_{15}H_{24}$	1449.3	1436.4	1639.1
δ-Elemene	Cyclohexene, 4-ethenyl-4-methyl-3-(1-methylethenyl)-1-(1-methylethyl)-, (3R-trans)-	20307-84-0	$C_{15}H_{24}$	1340.3	1337.0	1468.8
Elemicin	Benzene, 1,2,3-trimethoxy-5-(2-propenyl)-	487-11-6	$C_{12}H_{16}O_3$	1521.4	1553.6	2231.3
Elemol	Cyclohexanemethanol, 4-ethenyl-α,α,4-trimethyl-3-(1-methylethenyl)-, [1R-(1α,3α,4β)]-	639-99-6	$C_{15}H_{26}O$	1536.2	1547.5	2078.8
β-Elemol	Cyclohexanemethanol, 4-ethenyl-α,α,4-trimethyl-3-(1-methylethenyl)-, [1R-(1α,3β,4β)]-	32142-08-8	$C_{15}H_{26}O$	1537.2	[1548]	2087.7
4,5-Epoxy-2-decenal, (E)-	trans-4,5-Epoxy-(E)-2-decenal	134454-31-2	$C_{10}H_{16}O_2$	[1362]	1380.9	2000.7
Ethyl acetate	Acetic acid, ethyl ester	141-78-6	$C_4H_8O_2$	597.7	611.2	886.4
Ethyl benzoate	Benzoic acid, ethyl ester	93-89-0	$C_9H_{10}O_2$	1151.4	1171.3	1665.1
Ethyl butanoate	Butyric acid, ethyl ester	105-54-4	$C_6H_{12}O_2$	785.3	799.0	1035.7
Ethyl decanoate	Capric acid ethyl ester	110-38-3	$C_{12}H_{24}O_2$	1380.0	1395.0	1636.2
Ethyl dodecanoate	Lauric acid, ethyl ester	106-33-2	$C_{14}H_{28}O_2$	1578.2	1593.3	1839.7
Ethyl hexadecanoate	Palmitic acid, ethyl ester	628-97-7	$C_{18}H_{36}O_2$	1978.1	1991.5	2249.3
Ethyl hexanoate	Caproic acid ethyl ester	123-66-0	$C_8H_{16}O_2$	983.4	999.6	1233.4
Ethyl isovalerate	3-Methylbutanoic acid ethyl ester	108-64-5	$C_7H_{14}O_2$	836.1	853.1	1066.9
Ethyl linoleate	9,12-Octadecadienoic acid (Z,Z)-, ethyl ester	544-35-4	$C_{20}H_{36}O_2$	2150.5	2158.8	2521.9
Ethyl octanoate	Caprylic acid ethyl ester	106-32-1	$C_{10}H_{20}O_2$	1181.4	1196.2	1434.9
Ethyl pentanoate	Valeric acid, ethyl ester	539-82-2	$C_7H_{14}O_2$	882.9	901.2	1136.1
Ethyl tetradecanoate	Myristic acid, ethyl ester	124-06-1	$C_{16}H_{32}O_2$	1778.0	1793.9	2045.7
2-Ethylfuran		3208-16-0	C_6H_8O	689.1	704.6	953.2
Eudesm-7(11)-en-4-ol	1-Naphthalenol, decahydro-1,4a-dimethyl-7-(1-methylethylidene)-, [1R-(1α,4aβ,8aα)]-	473-04-1	$C_{15}H_{26}O$	1681.6	1692.3	[2302]
Eudesma-4(15),7-dien-1β-ol	1-Naphthalenol, 1,2,3,4,4a,5,8,8a-octahydro-8a-methyl-4-methylene-6-(1-methylethyl)-, [1R-(1α,4aβ,8aα)]-	119120-23-9	$C_{15}H_{24}O$	1675.8	1688.0	2371.3
α-Eudesmol	2-Naphthalenemethanol, 1,2,3,4,4a,5,6,8a-octahydro-α,α,4a,8-tetramethyl-, [2R-(2α,4aα,8aβ)]-	473-16-5	$C_{15}H_{26}O$	1641.1	1651.7	2222.7
β-Eudesmol	2-Naphthalenemethanol, 1,2α,3,4,4a,5,6,7,8,8aα-decahydro-α,α,4aβ-trimethyl-8-methylene-	473-15-4	$C_{15}H_{26}O$	1633.7	1650.1	2238.0
γ-Eudesmol	2-Naphthalenemethanol, 1,2,3,4,4a,5,6,7-octahydro-α,α,4a,8-tetramethyl-, (2R-cis)-	1209-71-8	$C_{15}H_{26}O$	1616.5	1630.9	2176.1
γ-Eudesmol, 10-epi-	2-Naphthalenemethanol, 1,2,3,4,4a,5,6,7-octahydro-α,α,4a,8-tetramethyl-, (2R-trans)-	15051-81-7	$C_{15}H_{26}O$	1607.9	1618.7	2105.8
Eugenol	Phenol, 2-methoxy-4-(2-propenyl)-	97-53-0	$C_{10}H_{12}O_2$	1339.6	1357.8	2162.7
Eugenol acetate	Phenol, 2-methoxy-4-(2-propenyl)-, acetate	93-28-7	$C_{12}H_{14}O_3$	1484.5	1523.7	2266.3

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TABLE 1. Cross-reference list of essential oil components (common names, other chemical identifiers and average retention index values)[a,b]—Continued

Name	Systematic name	CAS	Formula	RI(DIMS)	RI(DIMS5P)	RI(PEG)
β-Farnesene, (E)-	1,6,10-Dodecatriene, 7,11-dimethyl-3-methylene-, (E)-	18794-84-8	$C_{15}H_{24}$	1449.3	1455.9	1663.9
α-Farnesene, (E,E)-	1,3,6,10-Dodecatetraene, 3,7,11-trimethyl-, (E,E)-	502-61-4	$C_{15}H_{24}$	1496.3	1504.1	1743.9
α-Farnesene, (Z,E)-	1,3,6,10-Dodecatetraene, 3,7,11-trimethyl-, (Z,E)-	26560-14-5	$C_{15}H_{24}$	1480.6	1490.9	1727.9
β-Farnesene, cis-	1,6,10-Dodecatriene, 7,11-dimethyl-3-methylene-, (Z)-	28973-97-9	$C_{15}H_{24}$	1443.7	1445.9	1651.4
Farnesol, (2Z,6E)-	2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-, (Z,E)-	3790-71-4	$C_{15}H_{26}O$	1704.7	1722.5	2356.8
Farnesol, (2E,6E)	2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-, (E,E)-	106-28-5	$C_{15}H_{26}O$	1709.6	1743.5	[2366]
Farnesol, (2Z,6Z)-	2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-, (Z,Z)-	16106-95-9	$C_{15}H_{26}O$	1686.9	1694.4	2324.4
Farnesol, (2E,6Z)-	2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-, (E,Z)-	3879-60-5	$C_{15}H_{26}O$	1691.3	1713.6	[2341]
Farnesyl acetate, (2E,6E)-	2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-, acetate, (2E,6E)-	4128-17-0	$C_{17}H_{28}O_2$	1818.1	1842.3	2259.2
Farnesyl acetone, (5E,9E)	5,9,13-Pentadecatrien-2-one, 6,10,14-trimethyl-, (E,E)-	1117-52-8	$C_{18}H_{30}O$	1914.2	1919.5	[2377]
α-Fenchene	Bicyclo[2.2.1]heptane, 7,7-dimethyl-2-methylene-	471-84-1	$C_{10}H_{16}$	945.2	949.4	1061.0
Fenchol, endo-[c]	Bicyclo[2.2.1]heptan-2-ol, 1,3,3-trimethyl-, endo-	14575-74-7	$C_{10}H_{18}O$	1100.7	1115.1	1570.0
Fenchone[c]	1,3,3-Trimethylbicyclo[2.2.1]heptan-2-one	1195-79-5	$C_{10}H_{16}O$	1072.8	1087.6	1399.5
Fenchyl acetate, endo-	Bicyclo[2.2.1]heptan-2-ol, 1,3,3-trimethyl-, acetate, (1R,2R,4S)-rel-	4057-31-2	$C_{12}H_{20}O_2$	1209.0	1219.7	[1480]
Furaneol	2,5-Dimethyl-3-hydroxy-4-oxo-4,5-dihydrofuran	3658-77-3	$C_6H_8O_3$	1029.8	1072.3	2031.1
Furfural	2-Formylfuran	98-01-1	$C_5H_4O_2$	806.5	834.6	1460.9
Furfural, 5-methyl-	2-Formyl-5-methylfuran	620-02-0	$C_6H_6O_2$	933.3	967.3	1573.6
Furfuryl alcohol	2-(Hydroxymethyl)furan	98-00-0	$C_5H_6O_2$	832.2	862.6	1656.3
Geranial	2,6-Octadienal, 3,7-dimethyl-, (E)-	141-27-5	$C_{10}H_{16}O$	1247.1	1270.3	1725.0
Geraniol	2,6-Octadien-1-ol, 3,7-dimethyl-, (E)-	106-24-1	$C_{10}H_{18}O$	1238.9	1254.9	1839.3
Geranyl acetate	2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (E)-	105-87-3	$C_{12}H_{20}O_2$	1361.4	1379.9	1751.1
Geranyl butanoate	2,6-Octadien-1-ol, 3,7-dimethyl-, butyrate, (E)-	106-29-6	$C_{14}H_{24}O_2$	1537.1	1562.6	1879.0
Geranyl formate	2,6-Octadien-1-ol, 3,7-dimethyl-, formate, (2E)-	105-86-2	$C_{11}H_{18}O_2$	1282.5	1303.1	1696.9
Geranyl isobutanoate	Isobutyric acid, 3,7-dimethyl-2,6-octadienyl ester, (E)-	2345-26-8	$C_{14}H_{24}O_2$	1491.3	1514.4	1789.6
Geranyl isovalerate	Butanoic acid, 3-methyl-, (2E)-3,7-dimethyl-2,6-octadienyl ester	109-20-6	$C_{15}H_{26}O_2$	1587.5	1599.3	1904.1
Geranyl propanoate	2,6-Octadien-1-ol, 3,7-dimethyl-, propanoate, (E)-	105-90-8	$C_{13}H_{22}O_2$	1449.3	1476.8	1815.5
Geranyl tiglate	2-Butenoic acid, 2-methyl-, 3,7-dimethyl-2,6-octadienyl ester, (E,E)-	7785-33-3	$C_{15}H_{24}O_2$	1673.7	1700.8	2099.3
Geranylacetone	5,9-Undecadien-2-one, 6,10-dimethyl-, (E)-	3796-70-1	$C_{13}H_{22}O$	1431.1	1451.8	1854.9
Germacrene A	1,5-Cyclodecadiene, 1,5-dimethyl-8-(1-methylethenyl)-, [S-(E,E)]-	28387-44-2	$C_{15}H_{24}$	1490.6	1502.1	1747.4
Germacrene B	1,5-Cyclodecadiene, 1,5-dimethyl-8-(1-methylethylidene)-, (E,E)-	15423-57-1	$C_{15}H_{24}$	1535.1	1550.9	1823.8
Germacrene D	1,6-Cyclodecadiene, 1-methyl-5-methylene-8-(1-methylethyl)-, [S-(E,E)]-	23986-74-5	$C_{15}H_{24}$	1475.9	1480.6	1708.2
Germacrene-D-4-ol[c]	2,7-Cyclodecadien-1-ol, 1,7-dimethyl-4-(1-methylethyl)-, (2E,4S,7E)-	198991-79-6	$C_{15}H_{26}O$	1568.3	1574.2	2056.9
Gleenol	Spiro[4.5]dec-1-en-6-ol, 2,10-dimethyl-7-(1-methylethyl)-, [5S-(5α,6β,7β,10α)]-	72203-99-7	$C_{15}H_{26}O$	1574.2	1582.8	[2051]
Globulol	1H-Cycloprop[e]azulen-4-ol, decahydro-1,1,4,7-tetramethyl-, (1aα,4α,4aα,7α,7aβ,7bα)-	51371-47-2	$C_{15}H_{26}O$	1578.9	1581.8	2082.4
Globulol, epi-	1H-Cycloprop[e]azulen-4-ol, decahydro-1,1,4,7-tetramethyl-, [1aR-(1aα,4β,4aα,7α,7aβ,7bα)]-	88728-58-9	$C_{15}H_{26}O$	[1567]	1584.8	[2100]
o-Guaiacol	1-Hydroxy-2-methoxybenzene	90-05-1	$C_7H_8O_2$	1064.4	1092.1	1859.8
Guaiacol, 4-ethyl-	2-Methoxy-4-ethylphenol	2785-89-9	$C_9H_{12}O_2$	1253.6	1280.2	2029.9
Guaiacol, p-vinyl-	2-Methoxy-4-ethenylphenol	7786-61-0	$C_9H_{10}O_2$	1283.7	1317.4	2185.6
α-Guaiene	Azulene, 1,2,3,4,5,6,7,8-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1S-(1α,4α,7α)]-	3691-12-1	$C_{15}H_{24}$	1442.4	1439.6	[1652]
β-Guaiene, cis-	Azulene, 1,2,3,4,5,6,7,8-octahydro-1,4-dimethyl-7-(1-methylethylidene)-, (1S-cis)-	88-84-6	$C_{15}H_{24}$	1478.6	1488.8	1663.9
β-Guaiene, trans-	Azulene, 1,2,3,4,5,6,7,8-octahydro-1,4-dimethyl-7-(1-methylethylidene)-, trans-	192053-49-9	$C_{15}H_{24}$	1492.0	1499.2	[1532]
Guaiol	5-Azulenemethanol, 1,2,3,4,5,6,7,8-octahydro-α,α,3,8-tetramethyl-, [3S-(3α,5α,8α)]-	489-86-1	$C_{15}H_{26}O$	1588.9	1597.1	2088.9
α-Gurjunene	1H-Cycloprop[e]azulene, 1a,2,3,4,4a,5,6,7b-octahydro-1,1,4,7-tetramethyl-, [1aR-(1aα,4α,4aβ,7bα)]-	489-40-7	$C_{15}H_{24}$	1405.6	1408.6	1529.1

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TABLE 1. Cross-reference list of essential oil components (common names, other chemical identifiers and average retention index values)[a,b]—Continued

Name	Systematic name	CAS	Formula	RI(DIMS)	RI(DIMS5P)	RI(PEG)
β-Gurjunene	1H-Cyclopropa[a]naphthalene, 1a,2,3,5,6,7,7a,7b-octahydro-1,1,7,7a-tetramethyl-, (1aR,7R,7aR,7bS)-(+)-	17334-55-3	$C_{15}H_{24}$	1430.4	1431.2	1596.7
γ-Gurjunene	Azulene, 1,2,3,3a,4,5,6,7-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1R-(1α,3aβ,4α,7β)]-	22567-17-5	$C_{15}H_{24}$	1467.3	1472.2	1668.2
2-Heptadecanone		2922-51-2	$C_{17}H_{34}O$	1883.1	1903.4	2229.7
2,4-Heptadienal, (2E,4E)-		4313-03-5	$C_7H_{10}O$	982.6	1011.5	1491.0
Heptanal		111-71-7	$C_7H_{14}O$	880.7	902.0	1185.1
Heptanoic acid		111-14-8	$C_7H_{14}O_2$	1076.7	1080.1	1950.9
2-Heptanol		543-49-7	$C_7H_{16}O$	885.7	899.4	1315.3
1-Heptanol		111-70-6	$C_7H_{16}O$	955.5	968.6	1448.8
2-Heptanone	1-Methylhexanal	110-43-0	$C_7H_{14}O$	868.4	891.7	1182.3
5-Hepten-2-ol, 6-methyl-		1569-60-4	$C_8H_{16}O$	974.9	991.8	1463.8
2-Heptenal, (E)-		18829-55-5	$C_7H_{12}O$	930.5	960.5	1321.6
Hexadec-9-enoic acid, (Z)-	cis-Palmitoleic acid	373-49-9	$C_{16}H_{30}O_2$	1935.2	1951.1	[2944]
Hexadecanal	Palmitaldehyde	629-80-1	$C_{16}H_{32}O$	1797.1	1816.5	2132.0
Hexadecanoic acid	Palmitic acid	57-10-3	$C_{16}H_{32}O_2$	1955.4	1968.4	2913.2
1-Hexadecanol	1-Cetanol	36653-82-4	$C_{16}H_{34}O$	1861.6	1879.7	2374.9
2,4-Hexadienal-, (2E,4E)-	Sorbic aldehyde	142-83-6	C_6H_8O	879.2	913.2	1401.7
Hexahydrofarnesylacetone	6,10,14-Trimethyl-2-pentadecanone	502-69-2	$C_{18}H_{36}O$	1832.9	1844.4	2124.8
Hexanal	Caproic aldehyde	66-25-1	$C_6H_{12}O$	776.9	799.9	1082.0
Hexanoic acid	Caproic acid	142-62-1	$C_6H_{12}O_2$	985.1	996.4	1843.3
1-Hexanol	Caproyl alcohol	111-27-3	$C_6H_{14}O$	854.9	869.7	1351.4
1-Hexanol, 2-ethyl-		104-76-7	$C_8H_{18}O$	1015.3	1030.6	1487.9
2-Hexen-1-ol, (E)-		928-95-0	$C_6H_{12}O$	850.0	864.5	1399.9
3-Hexen-1-ol, (E)-		928-97-2	$C_6H_{12}O$	836.8	852.8	1372.8
3-Hexen-1-ol, (Z)-		928-96-1	$C_6H_{12}O$	842.3	856.6	1380.2
2-Hexen-1-ol, acetate, (E)-		2497-18-9	$C_8H_{14}O_2$	993.4	1011.5	1332.2
2-Hexenal, (E)-		6728-26-3	$C_6H_{10}O$	827.3	853.0	1216.3
3-Hexenal, (Z)-		6789-80-6	$C_6H_{10}O$	770.3	799.5	1139.1
3-Hexenyl acetate, (Z)-	3-Hexen-1-ol, acetate, (3Z)-	3681-71-8	$C_8H_{14}O_2$	985.9	1004.0	1315.9
3-Hexenyl benzoate, (Z)-		25152-85-6	$C_{13}H_{16}O_2$	1549.8	1569.5	2119.4
3-Hexenyl butanoate, (Z)-	Butanoic acid, 3-hexenyl ester, (Z)-	16491-36-4	$C_{10}H_{18}O_2$	1166.4	1184.7	1456.1
Hexyl 2-methyl butanoate	Butyric acid, 2-methyl-, hexyl ester	10032-15-2	$C_{11}H_{22}O_2$	1224.3	1236.3	1428.1
Hexyl acetate	Acetic acid, hexyl ester	142-92-7	$C_8H_{16}O_2$	995.9	1010.4	1273.5
Hexyl benzoate	Benzoic acid, hexyl ester	6789-88-4	$C_{13}H_{18}O_2$	1554.3	1581.8	2074.6
Hexyl butanoate	Butyric acid, hexyl ester	2639-63-6	$C_{10}H_{20}O_2$	1176.9	1191.5	1414.1
α-Himachalene	1H-Benzocycloheptene, 2,4a,5,6,7,8,9,9a-octahydro-3,5,5-trimethyl-9-methylene-, (4aS-cis)-	3853-83-6	$C_{15}H_{24}$	1444.8	1445.1	1663.9
β-Himachalene	1H-Benzocycloheptene, 2,4a,5,6,7,8-hexahydro-3,5,5,9-tetramethyl-, (R)-	1461-03-6	$C_{15}H_{24}$	1500.8	1501.0	1723.1
γ-Himachalene[c]	1H-Benzocycloheptene, 2,4a,5,6,7,9a-hexahydro-3,5,5,9-tetramethyl-, (4aS-cis)-	53111-25-4	$C_{15}H_{24}$	1471.2	1475.9	1708.7
Himachalol	1H-Benzocyclohepten-9-ol, 2,4a,5,6,7,8,9,9a-octahydro-3,5,5,9-tetramethyl-, [4aS-(4aα,9α,9aα)]-	1891-45-8	$C_{15}H_{26}O$	[1648]	1649.4	2240.8
Hotrienol[c]	1,5,7-Octatrien-3-ol, 3,7-dimethyl-, (E)-	53834-70-1	$C_{10}H_{16}O$	1087.6	1106.8	1602.5
α-Humulene	1,4,8-Cycloundecatriene, 2,6,6,9-tetramethyl-, (E,E,E)-	6753-98-6	$C_{15}H_{24}$	1449.3	1453.1	1666.7
β-Humulene	Cycloundecadiene, 1,4,4-trimethyl-8-methylene-, (E,E)-	116-04-1	$C_{15}H_{24}$	1448.0	1442.5	1673.2
Humulene epoxide II	12-Oxabicyclo[9.1.0]dodeca-3,7-diene, 1,5,5,8-tetramethyl-, (E,E)-(1R,11R)-(-)-	19888-34-7	$C_{15}H_{24}O$	1597.1	1604.7	2047.3
α-Humulene oxide	12-Oxabicyclo[9.1.0]dodeca-4,7-diene, 1,5,9,9-tetramethyl-, (E,E)-(1R,11R)-(-)-	19888-33-6	$C_{15}H_{24}O$	1590.7	1601.5	2019.6
Indole	2,3-Benzopyrrole	120-72-9	C_8H_7N	1273.3	1298.4	2440.5
Intermedeol	1-Naphthalenol, decahydro-1,4a-dimethyl-7-(1-methylethenyl)-, (1S,4aS,7R,8aS)-	6168-59-8	$C_{15}H_{26}O$	1636.1	1666.2	2243.0
α-Ionone, (E)-	3-Buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (E)-	127-41-3	$C_{13}H_{20}O$	1411.2	1425.6	1843.4

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TABLE 1. Cross-reference list of essential oil components (common names, other chemical identifiers and average retention index values)[a,b]—Continued

Name	Systematic name	CAS	Formula	RI(DIMS)	RI(DIMS5P)	RI(PEG)
β-Ionone, (E)-	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (E)-	79-77-6	$C_{13}H_{20}O$	1466.2	1485.9	1935.5
Isoborneol[c]	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, exo-	124-76-5	$C_{10}H_{18}O$	1147.8	1158.2	1659.1
Isobornyl acetate	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, acetate, exo-	125-12-2	$C_{12}H_{20}O_2$	1271.0	1285.9	1572.9
Isobutanol	1-Propanol, 2-methyl-	78-83-1	$C_4H_{10}O$	616.1	630.5	1089.3
α-Isocomene	Cyclopenta[c]pentalene, 1,2,3,3a,5a,6,7,8-octahydro-1,3a,4,5a-tetramethyl-, (1R,3aS,5aS,8aR)-	65372-78-3	$C_{15}H_{24}$	1388.1	1382.7	1388.1
iso-Dihydrocarveol	Cyclohexanol, 2-methyl-5-(1-methylethenyl)-, (1α,2β,5β)-	18675-35-9	$C_{10}H_{18}O$	[1212]	1213.4	[1800]
Isoitalicene	Cyclopenta[1,4]cyclobuta[1,2]benzene, 1,2,3,3a,4,4a,7,8-octahydro-1,4,4,6-tetramethyl-, (1R,3aR,4aR,8aR)-rel-(+)-	94482-89-0	$C_{15}H_{24}$	1378.0	1396.7	1490.5
Isomenthone	Cyclohexanone, 5-methyl-2-(1-methylethyl)-, cis-	491-07-6	$C_{10}H_{18}O$	1146.5	1159.1	1483.8
Isopentyl acetate	1-Butanol, 3-methyl-, acetate	123-92-2	$C_7H_{14}O_2$	858.4	875.0	1121.4
Isopentyl isovalerate	Butanoic acid, 3-methyl-, 3-methylbutyl ester	659-70-1	$C_{10}H_{20}O_2$	1088.4	1103.6	1293.8
Isophorone	1,1,3-Trimethyl-3-cyclohexene-5-one	78-59-1	$C_9H_{14}O$	1091.9	1127.2	1591.2
Isophytol	1-Hexadecen-3-ol, 3,7,11,15-tetramethyl-	505-32-8	$C_{20}H_{40}O$	1938.5	1946.8	2292.5
Isopulegone, trans-	Cyclohexanone, 5-methyl-2-(1-methylethenyl)-, trans-	29606-79-9	$C_{10}H_{16}O$	1155.6	1176.6	1596.2
Isospathulenol	1H-Cycloprop[e]azulen-7-ol, 1a,2,3,5,6,7,7a,7b-octahydro-1,1,4,7-tetramethyl-, [1aR-(1aα,7β,7aβ,7bα)]-	88395-46-4	$C_{15}H_{24}O$	1625.6	1633.5	2230.8
Isovaleric acid	Butanoic acid, 3-methyl-	503-74-2	$C_5H_{10}O_2$	826.3	860.4	1666.5
Italicene	Cyclopenta[1,4]cyclobuta[1,2]benzene, 1,2,3,3a,4,4a,7,8-octahydro-1,4,4,6-tetramethyl-, (1R,3aS,4aS,8aS)-rel-(-)-	94535-52-1	$C_{15}H_{24}$	1406.9	1401.9	[1543]
Jasmone, (Z)-	2-Cyclopenten-1-one, 3-methyl-2-(2-pentenyl)-, (Z)-	488-10-8	$C_{11}H_{16}O$	1368.9	1394.6	1955.2
4-Ketoisophorone	2,6,6-Trimethyl-2-cyclohexen-1,4-dione	1125-21-9	$C_9H_{12}O_2$	1104.1	1147.4	1682.5
Lavandulol	4-Hexen-1-ol, 2-isopropenyl-5-methyl-, (-)-	498-16-8	$C_{10}H_{18}O$	1155.0	1168.2	1679.4
Lavandulyl acetate	4-Hexen-1-ol, 5-methyl-2-(1-methylethenyl)-, acetate, (2R)-	20777-39-3	$C_{12}H_{20}O_2$	1273.2	1289.2	1602.3
Ledol	1H-Cycloprop[e]azulen-4-ol, decahydro-1,1,4,7-tetramethyl-, (1aS,4S,4aR,7S,7aR,7bR)-	577-27-5	$C_{15}H_{26}O$	1582.5	1566.8	2039.1
Limonen-4-ol	3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethenyl)-	3419-02-1	$C_{10}H_{16}O$	1158.2	1177.3	1688.1
Limonene[c]	1-Methyl-4-(1-methylethenyl)cyclohexene	138-86-3	$C_{10}H_{16}$	1023.7	1029.5	1198.2
Limonene oxide, cis-	7-Oxabicyclo[4.1.0]heptane, 1-methyl-4-(1-methylethenyl)-, (1α,4α,6α)-	13837-75-7	$C_{10}H_{16}O$	1117.9	1134.0	1450.5
Limonene oxide, trans-[c]	7-Oxabicyclo[4.1.0]heptane, 1-methyl-4-(1-methylethenyl)-, (1α,4β,6α)-	4959-35-7	$C_{10}H_{16}O$	1122.7	1137.5	1461.6
Linalool	3,7-Dimethyl-1,6-octadien-3-ol	78-70-6	$C_{10}H_{18}O$	1086.3	1099.0	1543.3
Linalool acetate	1,6-Octadien-3-ol, 3,7-dimethyl-, acetate	115-95-7	$C_{12}H_{20}O_2$	1242.3	1255.2	1554.0
Linalool oxide (pyranoid), trans-	2H-Pyran-3-ol, 6-ethenyltetrahydro-2,2,6-trimethyl-, trans-	39028-58-5	$C_{10}H_{18}O_2$	1161.8	1171.0	1738.5
Linalool oxide, (furanoid), cis-	2-Furanmethanol, 5-ethenyltetrahydro-α,α,5-trimethyl-, cis-	5989-33-3	$C_{10}H_{18}O_2$	1065.1	1075.1	1446.0
Linalool oxide, (furanoid), trans-	2-Furanmethanol, 5-ethenyltetrahydro-α,α,5-trimethyl-, trans-	34995-77-2	$C_{10}H_{18}O_2$	1072.3	1083.3	1454.3
Linalool propanoate	1,6-Octadien-3-ol, 3,7-dimethyl-, propanoate	144-39-8	$C_{13}H_{22}O_2$	1318.3	1336.0	[1604]
Linoleic acid	9,12-Octadecadienoic acid (Z,Z)-	60-33-3	$C_{18}H_{32}O_2$	2105.0	2128.9	[3290]
Longiborneol	1,4-Methanoazulen-9-ol, decahydro-1,5,5,8a-tetramethyl-, (1R,3aR,4S,8aS,9S)-(+)-	465-24-7	$C_{15}H_{26}O$	1592.2	1591.7	2157.2
Longicyclene	1,2,4-Methenoazulene, decahydro-1,5,5,8a-tetramethyl-, (1S,2R,3aR,4R,8aR,9S)-	1137-12-8	$C_{15}H_{24}$	1371.1	1376.9	1489.4
Longifolene	1,4-Methanoazulene, decahydro-4,8,8-trimethyl-9-methylene-, [1S-(1α,3aβ,4α,8aβ)]-	475-20-7	$C_{15}H_{24}$	1404.0	1406.8	1577.3
α-Longipinene	Tricyclo[5.4.0.02,8]undec-9-ene, 2,6,6,9-tetramethyl-, (1R,2S,7R,8R)-	5989-08-2	$C_{15}H_{24}$	1350.6	1352.1	[1469]
Manool	1-Naphthalenepropanol, α-ethenyldecahydro-α,5,5,8a-tetramethyl-2-methylene-, (αR,1S,4aS,8aS)-	596-85-0	$C_{20}H_{34}O$	2047.5	2057.3	[2628]

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TABLE 1. Cross-reference list of essential oil components (common names, other chemical identifiers and average retention index values)[a,b]—Continued

Name	Systematic name	CAS	Formula	RI(DIMS)	RI(DIMS5P)	RI(PEG)
Manool, 13-epi-	1H-Naphtho[2,1-b]pyran, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [3S-(3α,4aα,6aβ,10aα,10bβ)]-	1438-62-6	$C_{20}H_{34}O$	2008.3	2010.2	[2676]
Manoyl oxide	1H-Naphtho[2,1-b]pyran, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [3R-(3α,4aβ,6aα,10aβ,10bα)]-	596-84-9	$C_{20}H_{34}O$	1990.4	1993.1	[2376]
p-Menth-2-en-1-ol, cis-	2-Cyclohexen-1-ol, 1-methyl-4-(1-methylethyl)-, cis-	29803-82-5	$C_{10}H_{18}O$	1114.7	1123.1	1614.1
p-Menth-2-en-1-ol, trans-	2-Cyclohexen-1-ol, 1-methyl-4-(1-methylethyl)-, trans-	29803-81-4	$C_{10}H_{18}O$	1114.4	1136.7	1584.2
p-Mentha-1,5-dien-8-ol	2,4-Cyclohexadiene-1-methanol, α,α,4-trimethyl-	1686-20-0	$C_{10}H_{16}O$	1145.0	1166.6	[1674]
p-Mentha-2,8-dien-1-ol, cis-	2-Cyclohexen-1-ol, 1-methyl-4-(1-methylethenyl)-, cis-	3886-78-0	$C_{10}H_{16}O$	1117.1	1131.4	1652.1
p-Mentha-2,8-dien-1-ol, trans-	2-Cyclohexen-1-ol, 1-methyl-4-(1-methylethenyl)-, trans-	7212-40-0	$C_{10}H_{16}O$	1107.0	1127.5	[1639]
1(7),8-p-Menthadien-2-ol, cis-	Cyclohexanol, 2-methylene-5-(1-methylethenyl)-, cis-	22626-43-3	$C_{10}H_{16}O$	1202.5	1233.0	1894.9
1(7),8-p-Menthadien-2-ol, trans-	Cyclohexanol, 2-methylene-5-(1-methylethenyl)-, trans-	21391-84-4	$C_{10}H_{16}O$	1171.6	1180.5	1803.1
1,3,8-p-Menthatriene	1,3-Cyclohexadiene, 1-methyl-4-(1-methylethenyl)-	18368-95-1	$C_{10}H_{14}$	1100.7	1111.7	1411.0
Menthofuran	Benzofuran, 4,5,6,7-tetrahydro-3,6-dimethyl-	494-90-6	$C_{10}H_{14}O$	1152.7	1164.2	1482.4
Menthol[c]	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1α,2β,5α)-;	89-78-1	$C_{10}H_{20}O$	1162.7	1177.3	1630.4
Menthone[c]	Cyclohexanone, 5-methyl-2-(1-methylethyl)-, trans-	89-80-5	$C_{10}H_{18}O$	1136.9	1150.5	1465.3
Menthyl acetate	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, acetate, (1α,2β,5α)-	89-48-5	$C_{12}H_{22}O_2$	1281.4	1295.8	1554.8
Methional	Propionaldehyde, 3-(methylthio)-	3268-49-3	C_4H_8OS	866.2	907.5	1456.1
Methyl 3-phenylpropionate	3-Phenylpropanoic acid methyl ester	103-25-3	$C_{10}H_{12}O_2$	1246.5	1278.6	1854.5
p-Methyl anisole	1-Methoxy-4-methylbenzene	104-93-8	$C_8H_{10}O$	1001.9	1023.8	1431.7
Methyl benzoate	Benzoic acid, methyl ester	93-58-3	$C_8H_8O_2$	1073.9	1094.2	1615.5
Methyl chavicol	Benzene, 1-methoxy-4-(2-propenyl)-	140-67-0	$C_{10}H_{12}O$	1178.1	1195.8	1671.4
Methyl cinnamate, trans-	2-Propenoic acid, 3-phenyl-, methyl ester, (E)-	1754-62-7	$C_{10}H_{10}O_2$	1362.4	1375.4	2074.6
Methyl decanoate	Decanoic acid, methyl ester	110-42-9	$C_{11}H_{22}O_2$	1309.1	1325.5	1596.3
Methyl eugenol	Benzene, 1,2-dimethoxy-4-(2-propenyl)-	93-15-2	$C_{11}H_{14}O_2$	1376.1	1401.8	2006.3
Methyl geranate	Methyl 3,7-dimethyl-2,6-octadienoate	2349-14-6	$C_{11}H_{18}O_2$	1302.3	1323.1	1688.4
Methyl hexadecanoate	Palmitic acid, methyl ester	112-39-0	$C_{17}H_{34}O_2$	1909.4	1924.2	2210.6
Methyl hexanoate	Hexanoic acid, methyl ester	106-70-7	$C_7H_{14}O_2$	907.2	924.1	1184.6
Methyl linoleate	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	112-63-0	$C_{19}H_{34}O_2$	2078.8	2091.1	2493.8
Methyl octadecanoate	Stearic acid, methyl ester	112-61-8	$C_{19}H_{38}O_2$	2112.1	2126.7	2414.7
Methyl octanoate	Octanoic acid, methyl ester	111-11-5	$C_9H_{18}O_2$	1109.6	1127.5	1388.8
Methyl oleate	9-Octadecenoic acid (Z)-, methyl ester	112-62-9	$C_{19}H_{36}O_2$	2081.3	2096.1	2437.3
Methyl salicylate	2-Hydroxybenzoic acid methyl ester	119-36-8	$C_8H_8O_3$	1172.5	1192.9	1767.8
Methyl tetradecanoate	Myristic acid, methyl ester	124-10-7	$C_{15}H_{30}O_2$	1709.4	1723.3	1996.2
3-Methyl-1-butanol	Isopentyl alcohol	123-51-3	$C_5H_{12}O$	720.6	737.5	1206.9
6-Methyl-5-hepten-2-one	2-Methyl-2-heptene-6-ketone	110-93-0	$C_8H_{14}O$	964.4	985.9	1336.9
p-Methylacetophenone	1-(4-Methylphenyl)-1-ethanone	122-00-9	$C_9H_{10}O$	1161.4	1182.7	1773.8
3-Methylbutanal	Isovaleraldehyde	590-86-3	$C_5H_{10}O$	632.5	651.6	921.5
2-Methylpropyl 3-methylbutanoate	Isovaleric acid, isobutyl ester	589-59-3	$C_9H_{18}O_2$	989.3	1008.5	1186.4
Muurola-4 (14),5-diene, cis-	Naphthalene, 1,2,3,4,4a,5,6,7-octahydro-4-methyl-7-methylene-1-(1-methylethyl)-, [1S-(1α,4α,4aα)]-	157477-72-0	$C_{15}H_{24}$	1449.8	1463.6	[1643]
α-Muurolene[c]	Naphthalene, 1,2,4a,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1α,4aα,8aα)-	31983-22-9	$C_{15}H_{24}$	1491.0	1498.3	1723.4
γ-Muurolene	Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-7-methyl-4-methylene-1-(1-methylethyl)-, (1α,4aα,8aα)-	30021-74-0	$C_{15}H_{24}$	1473.0	1476.2	1689.8
α-Muurolol	1-Naphthalenol, 1,2,3,4,4a,7,8,8a-octahydro-1,6-dimethyl-4-(1-methylethyl)-, [1R-(1α,4β,4aβ,8aβ)]-	19435-97-3	$C_{15}H_{26}O$	1626.6	1642.9	2183.1
α-Muurolol, epi-	1-Naphthalenol, 1,2,3,4,4a,7,8,8a-octahydro-1,6-dimethyl-4-(1-methylethyl)-, [1S-(1α,4α,4aα,8aα)]-	19912-62-0	$C_{15}H_{26}O$	1631.2	1640.8	2186.4
Myrcene	3-Methylene-7-methyl-1,6-octadiene	123-35-3	$C_{10}H_{16}$	983.1	989.2	1160.9
Myrcenol	2-Methyl-6-methylene-7-octen-2-ol	543-39-5	$C_{10}H_{18}O$	1097.1	1113.1	[1585]
Myristicin	1,3-Benzodioxole, 4-methoxy-6-(2-propenyl)-	607-91-0	$C_{11}H_{12}O_3$	1494.4	1518.4	2261.4
Myrtenal[c]	6,6-Dimethylbicyclo[3.1.1]-hept-2-ene-2-carboxaldehyde	564-94-3	$C_{10}H_{14}O$	1170.8	1192.0	1631.5
Myrtenol	6,6-Dimethylbicyclo[3.1.1]hept-2-ene-2-methanol	515-00-4	$C_{10}H_{16}O$	1182.4	1194.1	1790.4

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TABLE 1. Cross-reference list of essential oil components (common names, other chemical identifiers and average retention index values)[a,b]—Continued

Name	Systematic name	CAS	Formula	RI(DIMS)	RI(DIMS5P)	RI(PEG)
Myrtenyl acetate	Bicyclo[3.1.1]hept-2-ene-2-methanol, 6,6-dimethyl-, acetate, (1S,5R)-	1079-01-2	$C_{12}H_{18}O_2$	1305.6	1328.6	1691.9
Naphthalene		91-20-3	$C_{10}H_8$	1164.6	1186.2	1735.6
neo-Menthol	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1α,2α,5β)-	491-01-0	$C_{10}H_{20}O$	1157.2	1167.4	1578.1
Nepetalactone, 4aα,7α,7aα	Cyclopenta[c]pyran-1(4aH)-one, 5,6,7,7a-tetrahydro-4,7-dimethyl-, [4aS-(4aα,7α,7aα)]-	21651-62-7	$C_{10}H_{14}O_2$	1326.7	1369.2	[1970]
Neral	2,6-Octadienal, 3,7-dimethyl-, (Z)-	106-26-3	$C_{10}H_{16}O$	1220.3	1242.1	1678.5
Nerol	2,6-Octadien-1-ol, 3,7-dimethyl-, (Z)-	106-25-2	$C_{10}H_{18}O$	1216.2	1228.9	1794.6
Nerol oxide	2H-Pyran, 3,6-dihydro-4-methyl-2-(2-methyl-1-propenyl)-	1786-08-9	$C_{10}H_{16}O$	1139.7	1154.7	1468.6
Nerolidol, (E)-	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, (E)-	40716-66-3	$C_{15}H_{26}O$	1550.1	1560.9	2036.3
Nerolidol, (Z)-[c]	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, (Z)-	3790-78-1	$C_{15}H_{26}O$	1524.4	1543.6	2007.3
Neryl acetate	2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (Z)-	141-12-8	$C_{12}H_{20}O_2$	1343.8	1362.9	1718.1
Neryl formate	2,6-Octadien-1-ol, 3,7-dimethyl-, formate, (Z)-	2142-94-1	$C_{11}H_{18}O_2$	1265.9	1285.0	1674.1
Neryl propanoate	2,6-Octadien-1-ol, 3,7-dimethyl-, propanoate, (Z)-	105-91-9	$C_{13}H_{22}O_2$	1430.6	[1452]	1777.7
2,4-Nonadienal, (2E,4E)-	trans-2,trans-4-Nonadienal	5910-87-2	$C_9H_{14}O$	1187.2	1215.8	1696.1
2,6-Nonadienal, (2E,6Z)-	2-trans-6-cis-Nonadienal	557-48-2	$C_9H_{14}O$	1125.9	1154.7	1582.2
γ-Nonalactone	Nonanoic acid, 4-hydroxy-, γ-lactone	104-61-0	$C_9H_{16}O_2$	1323.1	1363.5	2026.1
Nonanal		124-19-6	$C_9H_{18}O$	1083.8	1103.3	1391.5
Nonanoic acid	1-Octanecarboxylic acid	112-05-0	$C_9H_{18}O_2$	1268.9	1275.3	2159.1
2-Nonanol	1-Methyl-1-octanol	628-99-9	$C_9H_{20}O$	1089.8	1098.6	1519.6
1-Nonanol	1-Hydroxynonane	143-08-8	$C_9H_{20}O$	1157.2	1173.4	1655.7
2-Nonanone	Heptyl methyl ketone	821-55-6	$C_9H_{18}O$	1073.0	1092.5	1391.3
2-Nonenal, (E)-		18829-56-6	$C_9H_{16}O$	1135.6	1162.2	1535.9
2-Nonenal, (Z)-		60784-31-8	$C_9H_{16}O$	1125.3	1146.8	1501.9
Nonyl acetate	Acetic acid, nonyl ester	143-13-5	$C_{11}H_{22}O_2$	1293.8	1309.2	1578.6
Nootkatone	2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, [4R-(4α,4aα,6β)]-	4674-50-4	$C_{15}H_{22}O$	1776.5	1813.4	2548.3
Nopinone[c]	6,6-Dimethylbicyclo[3.1.1]heptan-2-one	24903-95-5	$C_9H_{14}O$	1106.8	1135.5	1573.1
β-Ocimene, (E)-	1,3,6-Octatriene, 3,7-dimethyl-, (E)-	3779-61-1	$C_{10}H_{16}$	1038.4	1047.7	1250.4
β-Ocimene, (Z)-	1,3,6-Octatriene, 3,7-dimethyl-, (Z)-	3338-55-4	$C_{10}H_{16}$	1028.9	1037.8	1234.5
Octadecanoic acid	Stearic acid	57-11-4	$C_{18}H_{36}O_2$	2158.7	2172.4	3148.3
1-Octadecanol	Stearic alcohol	112-92-5	$C_{18}H_{38}O$	2060.0	2082.8	2586.4
2,4-Octadienal-, (2E,4E)-		30361-28-5	$C_8H_{12}O$	1087.3	1113.9	1605.3
Octanal	Caprylaldehyde	124-13-0	$C_8H_{16}O$	982.4	1002.8	1287.2
Octanoic acid	Caprylic acid	124-07-2	$C_8H_{16}O_2$	1174.7	1182.0	2057.1
1-Octanol	Caprylic alcohol	111-87-5	$C_8H_{18}O$	1057.0	1071.5	1551.6
3-Octanol		589-98-0	$C_8H_{18}O$	983.8	993.2	1391.9
Octanol acetate	Acetic acid, octyl ester	112-14-1	$C_{10}H_{20}O_2$	1193.7	1209.3	1474.6
3-Octanone	Ethyl pentyl ketone	106-68-3	$C_8H_{16}O$	965.9	984.5	1254.8
2-Octen-1-ol, (E)-	trans-2-Octen-1-ol	18409-17-1	$C_8H_{16}O$	[1053.5]	1066.8	1610.3
1-Octen-3-ol		3391-86-4	$C_8H_{16}O$	965.9	980.0	1444.2
1-Octen-3-one	Amyl vinyl ketone	4312-99-6	$C_8H_{14}O$	955.9	978.0	1301.0
1-Octen-3-yl acetate	1-Pentylallyl acetate	2442-10-6	$C_{10}H_{18}O_2$	1091.3	1110.3	1379.7
2-Octenal (E)-	trans-2-Octenal	2548-87-0	$C_8H_{14}O$	1035.5	1060.2	1429.5
Oleic acid	9-Octadecenoic acid (Z)-	112-80-1	$C_{18}H_{34}O_2$	[2113]	2133.2	[3200]
β-Oplopenone	Ethanone, 1-[octahydro-4-methylene-7-(1-methylethyl)-1H-inden-1-yl]-, [1S-(1α,3aβ,7α,7aα)]-	28305-60-4	$C_{15}H_{24}O$	1592.9	1604.0	2084.5
Palustrol	4aH-Cycloprop[e]azulen-4a-ol, decahydro-1,1,4,7-tetramethyl-, [1aR-(1aα,4aβ,4aβ,7α,7aβ,7bα)]-	5986-49-2	$C_{15}H_{26}O$	1562.1	1566.8	1930.4
α-Patchoulene	1H-3a,7-Methanoazulene, 2,3,6,7,8,8a-hexahydro-1,4,9,9-tetramethyl-, (1α,3aα,7α,8aβ)-	560-32-7	$C_{15}H_{24}$	1451.3	1457.2	-
Patchouli alcohol	1,6-Methanonaphthalen-1(2H)-ol, octahydro-4,8a,9,9-tetramethyl-, [1R-(1α,4β,4aα,6β,8aα)]-	5986-55-0	$C_{15}H_{26}O$	1653.2	1659.8	[2156]
Pentadecanal		2765-11-9	$C_{15}H_{30}O$	1695.5	1714.4	[2041]
Pentadecanoic acid	Pentadecylic acid	1002-84-2	$C_{15}H_{30}O_2$	1853.8	1867.8	[2822]
2-Pentadecanone	Methyl tridecyl ketone	2345-28-0	$C_{15}H_{30}O$	1680.8	1699.1	2015.9
Pentanal	Valeraldehyde	110-62-3	$C_5H_{10}O$	675.4	700.3	975.3
1-Pentanol	Amyl alcohol	71-41-0	$C_5H_{12}O$	753.5	765.5	1247.1

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TABLE 1. Cross-reference list of essential oil components (common names, other chemical identifiers and average retention index values)[a,b]—Continued

Name	Systematic name	CAS	Formula	RI(DIMS)	RI(DIMS5P)	RI(PEG)
1-Penten-3-ol	1-Ethylallyl alcohol	616-25-1	$C_5H_{10}O$	665.7	690.1	1157.7
2-Pentenol, (Z)-	cis-2-Penten-1-ol	1576-95-0	$C_5H_{10}O$	746.8	771.2	1315.7
2-Pentylfuran	2-Amylfuran	3777-69-3	$C_9H_{14}O$	978.9	991.9	1232.1
Perilla alcohol	1-Cyclohexene-1-methanol, 4-(1-methylethenyl)-	536-59-4	$C_{10}H_{16}O$	1282.1	1296.3	2006.6
Perilla aldehyde	1-Cyclohexene-1-carboxaldehyde, 4-isopropenyl-	2111-75-3	$C_{10}H_{14}O$	1252.1	1273.4	1793.9
Perillene	Furan, 3-(4-methyl-3-pentenyl)-	539-52-6	$C_{10}H_{14}O$	1101.2	1098.6	1425.3
Phellandral	1-Cyclohexene-1-carboxaldehyde, 4-isopropyl-	21391-98-0	$C_{10}H_{16}O$	1250.1	1274.9	1723.9
α-Phellandrene	1,3-Cyclohexadiene, 2-methyl-5-(1-methylethyl)-	99-83-2	$C_{10}H_{16}$	999.1	1004.1	1167.7
β-Phellandrene	Cyclohexene, 3-methylene-6-(1-methylethyl)-	555-10-2	$C_{10}H_{16}$	1021.3	1030.0	1209.3
Phenol		108-95-2	C_6H_6O	956.6	983.3	1992.1
Phenylacetonitrile	(Cyanomethyl)benzene	140-29-4	C_8H_7N	1097.7	1146.5	1912.1
Phenylethyl 3-methylbutanoate	Isovaleric acid, phenethyl ester	140-26-1	$C_{13}H_{18}O_2$	1464.9	1490.5	1969.5
2-Phenylethyl acetate	Acetic acid, phenethyl ester	103-45-7	$C_{10}H_{12}O_2$	1229.7	1258.8	1812.9
2-Phenylethyl alcohol	Benzeneethanol	60-12-8	$C_8H_{10}O$	1088.2	1114.9	1903.7
β-Phenylethyl tiglate	2-Butenoic acid, 2-methyl-, 2-phenylethyl ester, (E)-	55719-85-2	$C_{13}H_{16}O_2$	1556.8	1590.0	[2210]
Phytol	2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-, (2E,7R,11R)-	150-86-7	$C_{20}H_{40}O$	2099.1	2116.4	2613.4
α-Pinene	2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	80-56-8	$C_{10}H_{16}$	934.5	936.1	1025.4
β-Pinene	6,6-Dimethyl-2-methylenebicyclo[3.1.1]heptane	127-91-3	$C_{10}H_{16}$	973.1	977.7	1110.0
Pinene hydrate, trans-	Bicyclo[3.1.1]heptan-2-ol, 2,6,6-trimethyl-, (1α,2β,5α)-	4948-29-2	$C_{10}H_{18}O$	1107.8	1121.2	[1522]
α-Pinene oxide	3-Oxatricyclo[4.1.1.02,4]octane, 2,7,7-trimethyl-	1686-14-2	$C_{10}H_{16}O$	1084.9	1097.0	1363.9
Pinocamphone, cis	Bicyclo[3.1.1]heptan-3-one, 2,6,6-trimethyl-, (1α,2β,5α)-	15358-88-0	$C_{10}H_{16}O$	1152.6	1172.8	1544.6
Pinocamphone, trans	Bicyclo[3.1.1]heptan-3-one, 2,6,6-trimethyl-, (1α,2α,5α)-	547-60-4	$C_{10}H_{16}O$	1143.9	1162.0	1523.4
Pinocarveol, trans-	Bicyclo[3.1.1]heptan-3-ol, 6,6-dimethyl-2-methylene-, [1S-(1α,3α,5α)]-	547-61-5	$C_{10}H_{16}O$	1126.2	1140.0	1661.2
Pinocarvone	Bicyclo[3.1.1]heptan-3-one, 6,6-dimethyl-2-methylene-	30460-92-5	$C_{10}H_{14}O$	1140.3	1160.6	1575.5
Piperitenone	2-Cyclohexen-1-one, 3-methyl-6-(1-methylethylidene)-	491-09-8	$C_{10}H_{14}O$	1316.9	1340.7	1909.1
Piperitenone oxide	7-Oxabicyclo[4.1.0]heptan-2-one, 6-methyl-3-(1-methylethylidene)-	35178-55-3	$C_{10}H_{14}O_2$	1342.3	1366.5	[1983]
Piperitol, cis-[c]	2-Cyclohexen-1-ol, 3-methyl-6-(1-methylethyl)-, cis-	16721-38-3	$C_{10}H_{18}O$	1186.3	1194.7	1750.5
Piperitol, trans-	2-Cyclohexen-1-ol, 3-methyl-6-(1-methylethyl)-, trans-	16721-39-4	$C_{10}H_{18}O$	1191.1	1205.3	1710.4
Piperitone	3-Methyl-6-isopropyl-2-cyclohexen-1-one	89-81-6	$C_{10}H_{16}O$	1232.7	1253.6	1729.9
Pulegone[c]	Cyclohexanone, 5-methyl-2-(1-methylethylidene)-, (R)-;	89-82-7	$C_{10}H_{16}O$	1222.7	1234.3	1654.5
Rose oxide, cis-[c]	2H-Pyran, tetrahydro-4-methyl-2-(2-methyl-1-propenyl)-, (2R,4S)-	4610-11-1	$C_{10}H_{18}O$	1096.4	1112.5	1350.1
Rose oxide, trans-[c]	2H-Pyran, tetrahydro-4-methyl-2-(2-methyl-1-propenyl)-, (2R,4R)-	5258-11-7	$C_{10}H_{18}O$	1115.7	1128.4	1367.3
Sabina ketone	Bicyclo[3.1.0]hexan-2-one, 5-isopropyl-	513-20-2	$C_9H_{14}O$	1141.0	1155.7	[1651]
Sabinene	1-Isopropyl-4-methylenebicyclo[3.1.0]hexane	3387-41-5	$C_{10}H_{16}$	967.9	973.0	1122.0
Sabinene hydrate acetate, cis-	Bicyclo[3.1.0]hexan-2-ol, 2-methyl-5-(1-methylethyl)-, acetate, (1α,2α,5α)-	77318-48-0	$C_{12}H_{20}O_2$	1212.5	1218.7	[1564]
Sabinene hydrate acetate, trans-	Bicyclo[3.1.0]hexan-2-ol, 2-methyl-5-(1-methylethyl)-, acetate, (1α,2β,5α)-	77318-47-9	$C_{12}H_{20}O_2$	1238.5	1253.4	[1610]
Sabinene hydrate, cis-	Bicyclo[3.1.0]hexan-2-ol, 2-methyl-5-(1-methylethyl)-, (1α,2α,5α)-	17699-16-0	$C_{10}H_{18}O$	1056.3	1066.5	1460.2
Sabinene hydrate, trans-	Bicyclo[3.1.0]hexan-2-ol, 2-methyl-5-(1-methylethyl)-, (1α,2β,5α)-	15826-82-1	$C_{10}H_{18}O$	1086.7	1098.1	1548.9
Sabinol, cis-	Bicyclo[3.1.0]hexan-3-ol, 4-methylene-1-(1-methylethyl)-, (1α,3α,5α)-	3310-02-9	$C_{10}H_{16}O$	1135.6	1142.4	1800.6
Sabinol, trans-	Bicyclo[3.1.0]hexan-3-ol, 4-methylene-1-(1-methylethyl)-, (1α,3β,5α)-	29606-76-6	$C_{10}H_{16}O$	1130.9	1139.2	1717.0
Safrole	Benzene, 4-allyl-1,2-(methylenedioxy)-	94-59-7	$C_{10}H_{10}O_2$	1271.2	1286.7	1868.1
Salicylaldehyde	2-Hydroxybenzaldehyde	90-02-8	$C_7H_6O_2$	1019.5	1046.5	1670.9
Salvial-4(14)-en-1-one	4(1H)-Azulenone, octahydro-3a-methyl-7-methylene-1-(1-methylethyl)-, [1S-(1α,3aα,8aα)]-;	73809-82-2	$C_{15}H_{24}O$	1584.7	1593.4	2035.9
α-Santalene[c]	Tricyclo[2.2.1.02,6]heptane, 1,7-dimethyl-7-(4-methyl-3-pentenyl)-, (-)-	512-61-8	$C_{15}H_{24}$	1415.9	1421.8	1582.7

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TABLE 1. Cross-reference list of essential oil components (common names, other chemical identifiers and average retention index values)[a,b]—Continued

Name	Systematic name	CAS	Formula	RI(DIMS)	RI(DIMS5P)	RI(PEG)
β-Santalene	Bicyclo[2.2.1]heptane, 2-methyl-3-methylene-2-(4-methyl-3-pentenyl)-, (1S,2R,4R)-	511-59-1	$C_{15}H_{24}$	1453.0	1458.5	1644.9
Santolina triene	1,4-Hexadiene, 2,5-dimethyl-3-vinyl-	2153-66-4	$C_{10}H_{16}$	903.3	907.4	1036.1
Selin-11-en-4α-ol	1-Naphthalenol, decahydro-1,4a-dimethyl-7-(1-methylethenyl)-, [1R-(1α,4aβ,7β,8aα)]-	16641-47-7	$C_{15}H_{26}O$	1641.1	1654.9	2252.0
Selina-3,7(11)-diene	Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-4a,8-dimethyl-2-(1-methylethylidene)-, (4aR-trans)-	6813-21-4	$C_{15}H_{24}$	1537.9	1540.5	1783.2
α-Selinene	Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-4a,8-dimethyl-2-(1-methylethenyl)-, [2R-(2α,4aα,8aβ)]-	473-13-2	$C_{15}H_{24}$	1489.5	1493.4	1725.3
β-Selinene	Naphthalene, decahydro-4a-methyl-1-methylene-7-(1-methylethenyl)-, [4aR-(4aα,7α,8aβ)]-	17066-67-0	$C_{15}H_{24}$	1480.7	1486.1	1716.9
α-Selinene, 7-epi-	Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-4a,8-dimethyl-2-(1-methylethenyl)-, [2S-(2α,4aβ,8aα)]-	123123-37-5	$C_{15}H_{24}$	1507.9	1517.2	1764.2
β-Sesquiphellandrene	Cyclohexene, 3-[(1S)-1,5-dimethyl-4-hexenyl]-6-methylene-, (3R)-	20307-83-9	$C_{15}H_{24}$	1513.2	1523.5	1771.4
Sesquisabinene hydrate, cis-	Bicyclo[3.1.0]hexan-2-ol, 5-[(1R)-1,5-dimethyl-4-hexenyl]-2-methyl-, (1S,2R,5R)-	58319-05-4	$C_{15}H_{26}O$	1534.8	1541.1	2081.5
Sesquisabinene hydrate, trans-	Bicyclo[3.1.0]hexan-2-ol, 5-(1,5-dimethyl-4-hexenyl)-2-methyl-, (1R,2R,5S)-rel-	145512-84-1	$C_{15}H_{26}O$	1584.4	1583.4	[2092]
α-Sinensal	2,6,9,11-Dodecatetraenal, 2,6,10-trimethyl-, (E,E,E)-	17909-77-2	$C_{15}H_{22}O$	1727.5	1753.5	2300.8
β-Sinensal	2,6,11-Dodecatrienal, 2,6-dimethyl-10-methylene-	60066-88-8	$C_{15}H_{22}O$	1669.6	1694.0	2229.3
Spathulenol	1H-Cycloprop[e]azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, [1aR-(1aα,4aα,7β,7aβ,7bα)]-	6750-60-3	$C_{15}H_{24}O$	1566.4	1576.4	2126.6
Styrene	Ethenylbenzene	100-42-5	C_8H_8	978.9	890.5	1261.5
Tagetone, (E)-	5,7-Octadien-4-one, 2,6-dimethyl-, (E)-	6752-80-3	$C_{10}H_{16}O$	[1123]	1127.3	[1501]
Tagetone, (Z)-	5,7-Octadien-4-one, 2,6-dimethyl-, (Z)-	3588-18-9	$C_{10}H_{16}O$	[1136]	1149.4	[1517]
Terpine-1-ol	1-Methyl-4-(1-methylethyl)-3-cyclohexen-1-ol	586-82-3	$C_{10}H_{18}O$	1134.0	1136.1	1572.9
Terpinen-4-ol	1-(1-Methylethyl)-4-methyl-3-cyclohexen-1-ol	562-74-3	$C_{10}H_{18}O$	1164.5	1177.1	1601.2
Terpinen-4-ol acetate	3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)-, acetate	4821-04-9	$C_{12}H_{20}O_2$	1283.1	1302.1	1640.1
α-Terpinene	1-Isopropyl-4-methyl-1,3-cyclohexadiene	99-86-5	$C_{10}H_{16}$	1010.9	1017.1	1177.8
γ-Terpinene	1-Isopropyl-4-methyl-1,4-cyclohexadiene	99-85-4	$C_{10}H_{16}$	1050.3	1059.7	1245.0
α-Terpineol	3-Cyclohexene-1-methanol, α,α,4-trimethyl-	98-55-5	$C_{10}H_{18}O$	1175.6	1189.7	1694.0
δ-Terpineol	Cyclohexanemethanol, α,α-dimethyl-4-methylene-	7299-42-5	$C_{10}H_{18}O$	1148.1	1164.5	1679.3
β-Terpineol, cis-	Cyclohexanol, 1-methyl-4-(1-methylethenyl)-, cis-	7299-41-4	$C_{10}H_{18}O$	1129.3	1143.9	[1639]
Terpinolene	4-Isopropylidene-1-methylcyclohexene	586-62-9	$C_{10}H_{16}$	1079.3	1086.9	1282.4
α-Terpinyl acetate	3-Cyclohexene-1-methanol, α,α,4-trimethyl-, acetate	80-26-2	$C_{12}H_{20}O_2$	1332.8	1347.0	1694.8
Tetradecanal	Myristaldehyde	124-25-4	$C_{14}H_{28}O$	1594.7	1612.3	1926.9
Tetradecanoic acid	Myristic acid	544-63-8	$C_{14}H_{28}O_2$	1753.3	1767.3	2686.8
1-Tetradecanol	Myristic alcohol	112-72-1	$C_{14}H_{30}O$	1663.1	1676.3	2152.4
Thuja-2,4(10)-diene	4-Methylene-1-(1-methylethyl)bicyclo[3.1.0]hex-2-ene	36262-09-6	$C_{10}H_{14}$	945.3	955.6	1122.0
α-Thujene	2-Methyl-5-isopropylbicyclo[3.1.0]-2-hexene	2867-05-2	$C_{10}H_{16}$	925.9	927.8	1026.6
Thujone, cis-	Bicyclo[3.1.0]hexan-3-one, 4-methyl-1-(1-methylethyl)-, [1S-(1α,4α,5α)]-	546-80-5	$C_{10}H_{16}O$	1090.9	1105.1	1423.1
Thujone, trans-	Bicyclo[3.1.0]hexan-3-one, 4-methyl-1-(1-methylethyl)-, [1S-(1α,4β,5α)]-	471-15-8	$C_{10}H_{16}O$	1098.4	1114.5	1439.6
Thujopsene, cis-	Cyclopropa[d]naphthalene, 1,1a,4,4a,5,6,7,8-octahydro-2,4a,8,8-tetramethyl-, (1aS,4aS,8aS)-(-)-	470-40-6	$C_{15}H_{24}$	1433.9	1432.0	1631.8
Thymol	1-Methyl-3-hydroxy-4-isopropylbenzene	89-83-8	$C_{10}H_{14}O$	1271.8	1290.1	2164.3
Thymol acetate	Phenol, 5-methyl-2-(1-methylethyl)-, acetate	528-79-0	$C_{12}H_{16}O_2$	1342.7	1356.4	[1867]
Thymol, methyl ether	1-Isopropyl-2-methoxy-4-methylbenzene	1076-56-8	$C_{11}H_{16}O$	1214.1	1234.3	1587.2
Tricyclene	1,7,7-Trimethyltricyclo[2.2.1.02,6]heptane	508-32-7	$C_{10}H_{16}$	921.9	923.2	1012.4
Tridecanal		10486-19-8	$C_{13}H_{26}O$	1491.1	1511.6	1818.5
Tridecanoic acid	Tridecylic acid	638-53-9	$C_{13}H_{26}O_2$	1659.1	1668.9	[2617]
2-Tridecanone	Methyl undecyl ketone	593-08-8	$C_{13}H_{26}O$	1478.8	1499.4	1808.1
Umbellulone	Bicyclo[3.1.0]hex-3-en-2-one, 4-methyl-1-(1-methylethyl)-	24545-81-1	$C_{10}H_{14}O$	1152.4	1171.4	1641.7
Undecanal	Undecylic aldehyde	112-44-7	$C_{11}H_{22}O$	1285.9	1306.5	1605.1
Undecanoic acid	Undecylic acid	112-37-8	$C_{11}H_{22}O_2$	1458.0	1474.4	2390.7
1-Undecanol	Undecyl alcohol	112-42-5	$C_{11}H_{24}O$	1357.9	1373.6	1853.3

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TABLE 1. Cross-reference list of essential oil components (common names, other chemical identifiers and average retention index values)[a,b]—Continued

Name	Systematic name	CAS	Formula	RI(DIMS)	RI(DIMS5P)	RI(PEG)
2-Undecanone	Methyl nonyl ketone	112-12-9	$C_{11}H_{22}O$	1275.6	1293.1	1598.1
2-Undecenal, (E)-	trans-2-Undecen-1-al	53448-07-0	$C_{11}H_{20}O$	1341.4	1364.6	1747.6
Valencene	Naphthalene, 1,2,3,5,6,7,8,8a-octahydro-1,8a-dimethyl-7-(1-methylethenyl)-, [1R-(1α,7β,8aα)]-	4630-07-3	$C_{15}H_{24}$	1483.0	1491.7	1728.6
Valeranone[c]	1(2H)-Naphthalenone, octahydro-4a,8a-dimethyl-7-(1-methylethyl)-, (4aα,7β,8aα)-	55528-90-0	$C_{15}H_{26}O$	1654.2	1671.8	2145.1
Vanillin	3-Methoxy-4-hydroxybenzaldehyde	121-33-5	$C_8H_8O_3$	1358.0	1404.7	2569.5
Veratrole	1,2-Dimethoxybenzene	91-16-7	$C_8H_{10}O_2$	1112.6	1148.1	1720.3
Verbenene	Bicyclo[3.1.1]hept-2-ene, 6,6-dimethyl-4-methylene-	4080-46-0	$C_{10}H_{14}$	945.7	963.3	1123.8
Verbenol, cis-[c]	Bicyclo[3.1.1]hept-3-en-2-ol, 4,6,6-trimethyl-, (1α,2β,5α)-	1845-30-3	$C_{10}H_{16}O$	1125.9	1144.4	1659.8
Verbenol, trans-	Bicyclo[3.1.1]hept-3-en-2-ol, 4,6,6-trimethyl-, (1α,2α,5α)-	1820-09-3	$C_{10}H_{16}O$	1133.7	1144.2	1680.3
Verbenone	4,6,6-Trimethylbicyclo[3.1.1]hept-3-en-2-one	80-57-9	$C_{10}H_{14}O$	1184.4	1206.2	1720.5
Viridiflorene	1H-Cycloprop[e]azulene, 1a,2,3,5,6,7,7a,7b-octahydro-1,1,4,7-tetramethyl-, [1aR-(1aα,7α,7aβ,7bα)]-	21747-46-6	$C_{15}H_{24}$	1488.9	1492.2	1696.2
Viridiflorol	1H-Cycloprop[e]azulen-4-ol, decahydro-1,1,4,7-tetramethyl-, [1aR-(1aα,4β,4aβ,7α,7aβ,7bα)]-	552-02-3	$C_{15}H_{26}O$	1579.9	1590.8	2089.8
α-Ylangene	Tricyclo[4.4.0.02,7]dec-3-ene, 1,3-dimethyl-8-(1-methylethyl)-, (1S,2R,6R,7R,8S)-	14912-44-8	$C_{15}H_{24}$	1370.0	1369.9	1484.1
β-Ylangene	Tricyclo[4.4.0.02,7]decane, 1-methyl-3-methylene-8-(1-methylethyl)-, (1R,2S,6S,7S,8R)-rel-	20479-06-5	$C_{15}H_{24}$	1416.3	1421.7	1576.9
Yomogi alcohol	3,6-Heptadien-2-ol, 2,5,5-trimethyl-, (E)-	26127-98-0	$C_{10}H_{18}O$	987.7	996.3	1395.1
α-Zingiberene	1,3-Cyclohexadiene, 5-[(1S)-1,5-dimethyl-4-hexenyl]-2-methyl-, (5R)-	495-60-3	$C_{15}H_{24}$	1482.9	1495.3	1720.7

[a]DIMS—dimethylsilicone, DIMS5P—dimethylsilicone with 5% phenyl groups, PEG—polyethylene glycol, CAS—Chemical Abstract Service registry number.
[b]RI estimates were provided in brackets for cross-reference purposes, when average values were not calculated.
[c]See Table 2 for related enantiomers or racemic mixtures.

TABLE 2. Related enantiomers and racemic mixtures

Component name	Related enantiomers and racemic mixtures (names and CAS Registry numbers)
α-Bisabolol	(-)-α-Bisabolol—23089-26-1; DL-α-Bisabolol—515-69-5
α-Bisabolol, epi-	(-)-epi-α-Bisabolol—78148-59-1
Borneol	(±)-Borneol—507-70-0; D-Borneol—464-43-7
α-Cadinene	(±)-α-Cadinene—82468-90-4; (-)-α-Cadinene—24406-05-1
Calamenene, cis-	(±)-cis-Calamenene—72937-55-4; (-)-cis-Calamenene—483-77-2
Camphene	DL-Camphene—79-92-5; D-Camphene—5794-03-6
Camphor	DL-Camphor—76-22-2; D-Camphor —464-49-3; L-Camphor—464-48-2
Carvone	DL-Carvone—99-49-0; L-Carvone 6485-40-1; D-Carvone—2244-16-8
Cuparene	(+)-Cuparene—16982-00-6; (-)-Cuparene—56324-31-3
γ-Elemene	(+)-γ-Elemene—30824-67-0
Fenchol, endo-	(-)-endo-Fenchol—512-13-0
Fenchone	(+)-Fenchone—4695-62-9; (±)- Fenchone—1195-79-5
Germacrene-D-4-ol	2,7-Cyclodecadien-1-ol, 1,7-dimethyl-4-(1-methylethyl)-, (1S,2E,4S,7E)-—74841-87-5; 2,7-Cyclodecadien-1-ol, 1,7-dimethyl-4-(1-methylethyl)-, (2E,4S,7E)-—198991-79-6
γ-Himachalene	(-)-γ-Himachalene—53111-25-4
Hotrienol	(±)-trans-Hotrienol—53834-70-1; (+)- Hotrienol—24278-80-6; (-)-trans-Hotrienol—20053-88-7
Isoborneol	DL-Isoborneol—124-76-5
Limonene	D-Limonene—5989-27-5; DL-Limonene—138-86-3; L-Limonene—5989-54-8
Limonene oxide, trans-	(D)-Limonene oxide, trans-—6909-30-4
Menthol	DL-Menthol—89-78-1; L-Menthol—2216-51-5; D-Menthol—15356-60-2
Menthone	DL-Menthone—89-80-5; D-Menthone—1196-31-2
α-Muurolene	(+)-α-Muurolene—17627-24-6; (-)-α-Muurolene—10208-80-7

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TABLE 2. Related enantiomers and racemic mixtures—Continued

Component name	Related enantiomers and racemic mixtures (names and CAS Registry numbers)
Myrtenal	(±)-Myrtenal—564-94-3; (-)-Myrtenal—18486-69-6
Nerolidol, (Z)-	(±)-cis-Nerolidol—3790-78-1; (+)-cis-Nerolidol—142-50-7
Nopinone	(-)-Nopinone—77982-63-9; (+)-Nopinone—38651-65-9
Piperitol, cis-	(±)-cis-Piperitol—16721-38-3; (+)-cis-Piperitol—34350-53-3
Pulegone	D-Pulegone—89-82-7; (-)-Pulegone—3391-90-0
Rose oxide, cis-	(+)-cis-Rose oxide—4610-11-1; (-)-cis-Rose oxide—3033-23-6; (±)-cis-Rose oxide—876-17-5
Rose oxide, trans-	(-)-trans-Rose oxide—5258-11-7; (±) trans-Rose oxide—876-18-6; (+)-trans-Rose oxide—5258-10-6
α-Santalene	(-)-α-Santalene—512-61-8; (±)-α-Santalene —27353-28-2
Valeranone	(±)-Valeranone—55528-90-0; (+)-Valeranone—1803-39-0; (-)-Valeranone—5090-54-0
Verbenol, cis-	(±)-cis-Verbenol—1845-30-3; (-)-cis-Verbenol—18881-04-4

TABLE 3. Retention indices of essential oil components for dimethylsilicone stationary phase

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
2,3-Butanedione	36	565.6	9.7	562	558–570	555–582	
Ethyl acetate	123	597.7	10.2	600	595–602	578–612	
Isobutanol	80	616.1	12.1	615	609–624	594–641	
Acetic acid	24	622.1	25.9	622	611–646	575–650	(d)
3-Methylbutanal	88	632.5	8.1	633	628–638	617–649	
Butanal, 2-methyl-	51	642.8	10.5	643	637–649	628–665	
1-Butanol	115	651.6	8.7	651	646–658	636–665	
1-Penten-3-ol	31	665.7	7.9	665	659–673	653–676	
Pentanal	72	675.4	7.7	675	671–679	664–692	
Acetoin	48	684.3	13.8	681.5	674–693	666–709	
2-Ethylfuran	17	689.1	7.2	690		676–705	
3-Methyl-1-butanol	114	720.6	9.4	719	716–725	706–738	
Butan-1-ol, 2-methyl-	52	721.9	7.3	722	718–726	709–735	
2-Pentenol, (Z)-	17	746.8	8.5	747		734–764	
2-Buten-1-ol, 3-methyl-	10	750.6	7.2	751.5		739–762	
1-Pentanol	113	753.5	9.9	753	740–770	747–760	
3-Hexenal, (Z)-	10	770.3	5.1	769.5		764–779	
Hexanal	201	776.9	6.7	776	772–779	769–788	
Ethyl butanoate	89	785.3	7.0	785	781–789	774–800	
Furfural	100	806.5	8.6	804	799–816	795–825	
Butanoic acid	22	806.8	18.9	806.5	795–823	778–830	
Isovaleric acid	24	826.3	18.7	826.5	806–841	803–855	
2-Hexenal, (E)-	109	827.3	7.1	827	824–830	817–844	
Butanoic acid, 2-methyl-	14	828.2	12.0	829		814–844	
Furfuryl alcohol	55	832.2	10.7	829	826–835	821–857	
Ethyl isovalerate	20	836.1	6.1	838	832–840	824–844	
3-Hexen-1-ol, (E)-	46	836.8	10.3	836	830–844	823–853	
3-Hexen-1-ol, (Z)-	129	842.3	10.1	840	834–848	829–862	
2-Hexen-1-ol, (E)-	71	850.0	7.3	849	845–855	840–862	
1-Hexanol	155	854.9	11.3	854	849–859	837–878	
Isopentyl acetate	65	858.4	4.9	859	855–861	851–866	
Methional	37	866.2	6.0	865	862–870	856–875	
2-Heptanone	106	868.4	6.0	869	865–872	859–877	
2,4-Hexadienal-, (2E,4E)-	11	879.2	3.1	878		876–884	
Heptanal	112	880.7	6.3	879	877–883	873–897	
Ethyl pentanoate	35	882.9	5.4	883	880–887	875–891	
2-Acetylfuran	55	883.8	7.3	884	878–889	875–896	
2-Heptanol	48	885.7	5.2	886	882–888	879–894	
Santolina triene	12	903.3	2.9	903		900–910	
Methyl hexanoate	71	907.2	3.1	907	905–909	902–914	

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TABLE 3. Retention indices of essential oil components for dimethylsilicone stationary phase—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
Tricyclene	92	921.9	8.4	921	918–926	908–936	
α-Thujene	297	925.9	6.5	924	922–930	916–938	
2-Heptenal, (E)-	31	930.5	4.6	930	927–932	926–941	
Furfural, 5-methyl-	55	933.3	7.0	933	927–937	924–946	
α-Pinene	569	934.5	8.3	933	930–938	924–951	
Benzaldehyde	208	936.6	13.8	933	926–945	921–965	
α-Fenchene	41	945.2	7.5	944	941–950	937–959	
Thuja-2,4(10)-diene	12	945.3	7.1	943		937–957	
Verbenene	14	945.7	3.8	946		937–953	
Camphene	356	947.4	9.1	946	941–953	936–965	
Dimethyl trisulfide	57	948.3	8.4	949	941–952	935–964	
1-Heptanol	75	955.5	9.3	954	951–960	941–974	
1-Octen-3-one	23	955.9	4.1	956	953–958	952–962	
Phenol	97	956.6	12.2	956	950–964	932–979	
6-Methyl-5-hepten-2-one	98	964.4	7.9	964	961–968	942–973	
1-Octen-3-ol	122	965.9	6.9	964	961–970	958–980	
3-Octanone	37	965.9	3.2	966	964–969	961–971	
Sabinene	376	967.9	7.5	967	963–972	958–981	
β-Pinene	485	973.1	8.3	972	968–978	962–987	
5-Hepten-2-ol, 6-methyl-	4	974.9	1.2			974–977	
2-Pentylfuran	63	978.9	3.4	979	977–981	973–984	
Styrene	78	978.9	7.7	878	873–884	870–896	
Dehydro-1,8-cineole	25	979.8	4.9	980	975–982	973–989	
Octanal	157	982.4	4.9	981	979–985	975–992	
2,4-Heptadienal, (2E,4E)-	24	982.6	8.1	982.5	979–988	967–994	
Myrcene	482	983.1	5.0	983	981–986	975–991	
Ethyl hexanoate	80	983.4	5.3	982	980–986	976–993	
3-Octanol	47	983.8	6.0	984	980–986	974–995	
Hexanoic acid	38	985.1	18.1	983	973–1005	951–1010	
3-Hexenyl acetate, (Z)-	55	985.9	5.8	986	984–988	977–996	
Yomogi alcohol	10	987.7	4.1	988		982–996	
2-Methylpropyl 3-methylbutanoate	15	989.3	2.8	989		985–994	
2-Hexen-1-ol, acetate, (E)-	10	993.4	4.2	995		983–997	
Hexyl acetate	96	995.9	8.4	995	991–1001	984–1012	
δ-2-Carene	33	997.7	9.5	998	991–1003	983–1013	
α-Phellandrene	289	999.1	6.5	998	995–1002	990–1009	
p-Methyl anisole	19	1001.9	7.0	1003		986–1015	
3-Carene	186	1007.2	9.2	1005	1001–1010	997–1027	
1,4-Cineole	19	1008.9	4.9	1010		998–1019	
α-Terpinene	296	1010.9	8.1	1010	1007–1013	1001–1024	
m-Cymene	44					998–1037	(e)
p-Cymene	528	1015.1	7.7	1014	1010–1018	1004–1029	(e)
1-Hexanol, 2-ethyl-	30	1015.3	3.1	1015	1013–1018	1010–1020	
Benzyl alcohol	105	1015.4	13.4	1009	1005–1025	1002–1040	
Benzeneacetaldehyde	104	1016.1	21.5	1011	1006–1018	1002–1043	
Salicylaldehyde	15	1019.5	10.3	1024		1003–1031	
β-Phellandrene	188	1021.3	9.4	1021	1018–1026	1005–1036	
1,8-Cineole	348	1022.4	8.8	1022	1018–1026	1013–1039	
Limonene	599	1023.7	7.6	1023	1020–1027	1012–1038	
β-Ocimene, (Z)-	272	1028.9	6.8	1028	1025–1032	1017–1040	
Furaneol	19	1029.8	7.4	1029		1023–1049	
o-Cymene	37					1009–1076	(e)
2-Octenal, (E)-	30	1035.5	4.9	1034	1031–1040	1030–1045	
β-Ocimene, (E)-	303	1038.4	6.3	1038	1035–1042	1027–1050	
Acetophenone	94	1041.5	12.5	1040	1031–1047	1027–1067	
Artemisia ketone	16	1048.3	9.1	1045		1039–1069	
γ-Terpinene	412	1050.3	7.3	1050	1047–1055	1035–1062	

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TABLE 3. Retention indices of essential oil components for dimethylsilicone stationary phase—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
p-Cresol	54	1051.7	8.7	1052	1048–1056	1035–1065	
2-Octen-1-ol, (E)-	2					1052–1055	
Sabinene hydrate, cis-	135	1056.3	6.8	1056	1052–1060	1044–1066	(f)
1-Octanol	169	1057.0	8.3	1057	1053–1061	1048–1073	
o-Guaiacol	53	1064.4	10.8	1059	1057–1071	1053–1087	
Linalool oxide, (furanoid), cis-	119	1065.1	8.8	1064	1058–1068	1054–1081	
Artemisia alcohol	14	1071.5	5.1	1072		1064–1082	
Linalool oxide, (furanoid), trans-	113	1072.3	9.5	1074	1067–1078	1055–1085	
Fenchone	55	1072.8	9.4	1072	1066–1080	1059–1087	
2-Nonanone	72	1073.0	9.5	1072	1069–1077	1058–1093	
p-Cymenene	72	1073.7	5.5	1073	1071–1078	1066–1082	
Methyl benzoate	75	1073.9	10.7	1071	1065–1081	1062–1096	
Heptanoic acid	14	1076.7	14.1	1078		1049–1103	(d)
Terpinolene	352	1079.3	7.2	1079	1076–1083	1064–1091	
Nonanal	193	1083.8	6.3	1083	1081–1086	1073–1097	
α-Pinene oxide	12	1084.9	11.6	1087		1060–1100	
Linalool	551	1086.3	7.6	1086	1083–1089	1074–1098	
Sabinene hydrate, trans-	100	1086.7	11.6	1087	1079–1094	1070–1107	(f)
2,4-Octadienal-, (2E,4E)-	4	1087.3	1.9			1086–1090	
Hotrienol	7	1087.6	2.4	1089		1085–1090	
2-Phenylethyl alcohol	134	1088.2	10.2	1086	1080–1095	1076–1105	
Isopentyl isovalerate	19	1088.4	5.5	1090		1080–1100	
2-Nonanol	15	1089.8	7.2	1087		1084–1109	
Thujone, cis-	43	1090.9	8.8	1090	1086–1098	1076–1104	
1-Octen-3-yl acetate	14	1091.3	4.8	1093		1083–1100	
Isophorone	26	1091.9	9.4	1089	1086–1097	1081–1112	
Rose oxide, cis-	18	1096.4	2.2	1097		1092–1100	
Myrcenol	15	1097.1	9.9	1100		1076–1111	
Phenylacetonitrile	16	1097.7	7.7	1098		1084–1111	
Thujone, trans-	25	1098.4	9.2	1098	1093–1100	1086–1115	
Fenchol, endo-	32	1100.7	9.4	1100	1094–1104	1088–1122	
1,3,8-p-Menthatriene	11	1100.7	13.7	1104		1074–1118	
Perillene	11	1101.2	11.2	1099		1086–1119	(d)
4-Ketoisophorone	6	1104.1	9.0	1105		1090–1117	
Chrysanthenone	16	1104.3	7.5	1103		1092–1122	
α-Campholenal	57	1106.8	9.4	1105	1102–1113	1094–1126	
Nopinone	11	1106.8	11.0	1108		1087–1129	
p-Mentha-2,8-dien-1-ol, trans-	12	1107.0	4.2	1108		1098–1111	
Pinene hydrate, trans-	7	1107.8	7.5	1103		1097–1130	
Methyl octanoate	65	1109.6	5.5	1108	1107–1110	1105–1122	
Veratrole	13	1112.6	4.5	1111		1109–1126	
p-Menth-2-en-1-ol, trans-	56	1114.4	11.2	1112	1108–1123	1095–1130	
p-Menth-2-en-1-ol, cis-	49	1114.7	11.4	1114	1106–1126	1099–1130	
Rose oxide, trans-	16	1115.7	7.1	1115		1107–1130	
allo-Ocimene	25	1116.4	8.6	1116	1111–1118	1102–1133	
p-Mentha-2,8-dien-1-ol, cis-	19	1117.1	6.9	1117		1100–1127	
Limonene oxide, cis-	28	1117.9	6.7	1118.5	1116–1122	1102–1126	
Limonene oxide, trans-	29	1122.7	5.8	1124	1121–1125	1110–1130	
Tagetone, (E)-	6					1120–1136	(g); 1132 (Ref. 50); 1135 (Ref. 51)
Camphor	222	1125.0	13.1	1123.5	1118–1130	1106–1153	
2-Nonenal, (Z)-	8	1125.3	6.0	1123		1118–1133	
2,6-Nonadienal, (2E,6Z)-	21	1125.9	8.1	1124	1122–1127	1117–1145	
Verbenol, cis-	35	1125.9	10.3	1126	1120–1131	1110–1146	
Pinocarveol, trans-	72	1126.2	10.8	1126	1119–1131	1106–1143	
β-Terpineol, cis-	6	1129.3	4.3	1129		1125–1137	
Sabinol, trans-	13	1130.9	8.3	1131		1120–1148	

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TABLE 3. Retention indices of essential oil components for dimethylsilicone stationary phase—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
Citronellal	67	1133.6	5.2	1133	1130–1137	1126–1143	
Verbenol, trans-	61	1133.7	12.6	1131	1125–1144	1114–1157	
Terpine-1-ol	8	1134.0	10.7			1120–1147	
2-Nonenal, (E)-	56	1135.6	6.0	1134.5	1132–1139	1127–1147	
Sabinol, cis-	10	1135.6	6.9	1133.5		1128–1147	
Camphene hydrate	18	1135.8	7.8	1134.5		1127–1152	
Tagetone, (Z)-	11					1124–1156	(g); 1140 (Ref. 44); 1147 (Ref. 45)
Menthone	72	1136.9	8.3	1136.5	1131–1142	1125–1150	
1,4-Dimethoxybenzene	10	1138.4	16.1	1131		1122–1171	
Nerol oxide	12	1139.7	2.7	1139		1136–1144	
Pinocarvone	65	1140.3	10.4	1140	1135–1145	1121–1158	
Sabina ketone	5	1141.0	9.8			1126–1151	
Benzyl acetate	46	1141.1	11.2	1138.5	1134–1145	1128–1163	
Pinocamphone, trans	19	1143.9	9.4	1141		1134–1163	
p-Mentha-1,5-dien-8-ol	18	1145.0	8.4	1143		1131–1165	
Isomenthone	37	1146.5	7.7	1148	1143–1151	1130–1157	
Isoborneol	49	1147.8	8.8	1149	1142–1156	1131–1160	
δ-Terpineol	29	1148.1	10.5	1146	1142–1153	1134–1166	
Chrysanthenol, cis-	9	1150.3	3.5	1152		1146–1155	
Ethyl benzoate	73	1151.4	10.2	1149	1143–1156	1139–1175	
Umbellulone	8	1152.4	8.3	1152		1142–1165	
Pinocamphone, cis	18	1152.6	4.6	1151.5		1146–1160	
Menthofuran	12	1152.7	10.4	1151		1135–1175	
Borneol	250	1153.2	10.7	1152	1147–1157	1134–1172	
Lavandulol	39	1155.0	7.2	1153	1150–1160	1145–1168	
Isopulegone, trans-	5	1155.6	2.6	1155		1152–1159	
Cryptone	26	1156.7	7.2	1156.5	1150–1163	1148–1165	
1-Nonanol	64	1157.2	6.1	1157	1154–1161	1147–1166	
neo-Menthol	19	1157.2	4.4	1157		1151–1169	
Limonen-4-ol	5	1158.2	7.8	1157		1151–1169	
p-Methylacetophenone	21	1161.4	8.5	1160	1157–1164	1151–1179	
Linalool oxide (pyranoid), trans-	11	1161.8	9.4	1164		1147–1176	
Menthol	62	1162.7	9.4	1165	1155–1170	1148–1177	
p-Cresol, 2-methoxy-	14	1163.4	6.3	1162		1155–1181	
Terpinen-4-ol	440	1164.5	9.3	1163.5	1159–1170	1148–1180	
p-Cymen-8-ol	86	1164.6	10.0	1162	1158–1169	1148–1184	
Naphthalene	136	1164.6	15.2	1161	1154–1173	1142–1196	
3-Hexenyl butanoate, (Z)-	35	1166.4	5.4	1167	1165–1170	1154–1174	
Myrtenal	81	1170.8	9.0	1171	1165–1175	1153–1188	
1(7),8-p-Menthadien-2-ol, trans-	8	1171.6	4.2	1174		1165–1175	
Methyl salicylate	73	1172.5	9.3	1172	1166–1179	1160–1192	
Octanoic acid	33	1174.7	17.0	1175	1158–1187	1153–1202	
α-Terpineol	465	1175.6	9.3	1175	1170–1180	1159–1191	
Hexyl butanoate	42	1176.9	4.1	1176	1175–1178	1173–1185	
Cinnamaldehyde, cis-	5	1178.0	12.7			1161–1198	
Methyl chavicol	50	1178.1	7.5	1177	1174–1181	1169–1190	
Ethyl octanoate	54	1181.4	5.3	1180	1179–1183	1175–1193	
Dihydrocarveol	18	1181.9	5.1	1181		1174–1191	
Myrtenol	94	1182.4	8.9	1181.5	1177–1186	1169–1200	
Verbenone	61	1184.4	9.3	1184	1178–1191	1167–1198	
Dihydrocarvone, trans-	11	1184.9	13.6	1187		1162–1206	
Decanal	159	1185.7	6.3	1185	1183–1188	1177–1201	
Piperitol, cis-	29	1186.3	7.9	1185	1182–1190	1176–1201	
2,4-Nonadienal, (2E,4E)-	16	1187.2	4.2	1187.5		1180–1194	
Piperitol, trans-	29	1191.1	7.5	1192	1187–1195	1180–1205	
Octanol acetate	79	1193.7	4.7	1193	1191–1196	1188–1199	

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TABLE 3. Retention indices of essential oil components for dimethylsilicone stationary phase—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
β-Cyclocitral	29	1196.1	3.8	1196	1194–1200	1189–1202	
Carveol, trans-	84	1200.9	8.7	1199	1195–1208	1189–1215	
1(7),8-p-Menthadien-2-ol, cis-	6	1202.5	3.6	1204		1198–1206	
Carveol, cis-	44	1206.4	8.4	1206	1200–1210	1196–1224	
Bornyl formate	3					1199–1208	1208 (Ref. 46)
Fenchyl acetate, endo-	4	1209.0	4.5	1208		1205–1215	
iso-Dihydrocarveol	3					1151–1212	1212 (Ref. 47)
Citronellol	121	1212.4	5.6	1211	1208–1215	1207–1225	
Sabinene hydrate acetate, cis-	8	1212.5	3.3	1213.5		1209–1218	
Cumin aldehyde	48	1212.6	9.5	1215	1204–1219	1196–1226	
Thymol, methyl ether	55	1214.1	9.3	1214	1208–1217	1199–1235	
Nerol	144	1216.2	10.3	1213	1209–1219	1206–1239	
Carvone	108	1218.0	9.2	1218	1212–1224	1206–1235	
Neral	108	1220.3	9.5	1217	1214–1223	1211–1240	
Carvotanacetone	6	1221.0	8.7	1219.5		1213–1236	
Carvacrol, methyl ether	36	1221.5	7.1	1224	1219–1225	1205–1230	
Pulegone	52	1222.7	11.6	1220	1215–1230	1208–1248	
p-Anisaldehyde	37	1222.7	12.7	1221	1211–1234	1206–1240	
Hexyl 2-methyl butanoate	12	1224.3	3.6	1224		1218–1232	
2-Phenylethyl acetate	37	1229.7	8.1	1228	1224–1233	1221–1245	
Piperitone	78	1232.7	8.5	1232.5	1228–1236	1221–1249	
Chavicol	13	1236.9	7.6	1234		1226–1252	
Sabinene hydrate acetate, trans-	12	1238.5	7.2	1239.5		1226–1249	
Cinnamaldehyde, trans-	16	1238.6	13.8	1235		1222–1266	
Geraniol	218	1238.9	7.6	1237	1234–1242	1231–1256	
2-Decenal, (E)-	36	1239.1	4.2	1239.5	1236–1242	1232–1246	
Linalool acetate	106	1242.3	6.2	1241	1239–1245	1234–1254	
Methyl 3-phenylpropionate	10	1246.5	5.8	1245.5		1239–1258	
Geranial	126	1247.1	7.9	1247	1242–1252	1236–1260	
Chrysanthenyl acetate, cis-	17	1248.4	6.3	1248		1238–1260	
p-Anisyl alcohol	5	1249.7	9.9			1242–1267	1240–1247 (Ref. 40)
Phellandral	12	1250.1	6.6	1251		1237–1259	
Perilla aldehyde	37	1252.1	8.2	1252	1246–1255	1241–1271	
Guaiacol, 4-ethyl-	15	1253.6	10.2	1250		1243–1278	
1-Decanol	65	1258.5	7.9	1257	1255–1262	1247–1275	
Citronellyl formate	21	1260.4	2.9	1261	1260–1261	1255–1263	
Anethole, (E)-	53	1264.7	9.6	1264	1258–1271	1253–1284	
Neryl formate	14	1265.9	4.7	1267		1256–1272	
Nonanoic acid	28	1268.9	13.7	1268.5	1260–1279	1249–1291	
p-Cymen-7-ol	25	1270.1	8.3	1270	1265–1275	1260–1283	
Bornyl acetate	172	1270.2	8.2	1270	1265–1274	1259–1284	
Isobornyl acetate	28	1271.0	7.7	1271	1265–1278	1259–1282	
Safrole	31	1271.2	10.2	1269	1264–1278	1258–1289	
Thymol	179	1271.8	8.8	1270	1266–1276	1260–1289	
2,4-Decadienal, (2E,4Z)-	22	1273.1	8.1	1272.5	1268–1279	1260–1288	
Lavandulyl acetate	31	1273.2	2.5	1273	1272–1275	1268–1276	
Indole	43	1273.3	17.2	1271	1261–1280	1248–1304	
2-Undecanone	56	1275.6	6.4	1274	1272–1277	1269–1289	
Menthyl acetate	24	1281.4	7.8	1281	1278–1284	1268–1294	
Perilla alcohol	26	1282.1	8.2	1281	1276–1287	1274–1299	
Geranyl formate	28	1282.5	4.1	1282	1280–1284	1277–1289	
Carvacrol	113	1282.7	9.3	1278	1275–1289	1272–1300	
Terpinen-4-ol acetate	9	1283.1	10.1	1282		1270–1302	
Guaiacol, p-vinyl-	28	1283.7	7.2	1280	1280–1289	1274–1298	
Undecanal	63	1285.9	6.2	1287	1285–1289	1274–1294	
2,4-Decadienal, (2E,4E)-	68	1290.5	7.7	1288	1287–1293	1282–1304	
Nonyl acetate	20	1293.8	4.8	1292	1291–1295	1290–1302	

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TABLE 3. Retention indices of essential oil components for dimethylsilicone stationary phase—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
Methyl geranate	19	1302.3	3.2	1302		1298–1308	
Myrtenyl acetate	16	1305.6	7.3	1306		1290–1316	
Methyl decanoate	52	1309.1	4.4	1307	1306–1311	1305–1320	
Piperitenone	10	1316.9	6.5	1316		1304–1324	
Linalool propanoate	12	1318.3	4.3	1318.5		1312–1324	
Carvyl acetate, trans-	11	1321.9	7.1	1326		1312–1331	
γ-Nonalactone	30	1323.1	9.0	1324	1317–1330	1308–1337	
Nepetalactone, 4aα,7α,7aα	7	1326.7	9.8	1322		1317–1344	
α-Terpinyl acetate	112	1332.8	7.6	1333	1330–1334	1324–1348	
Carvyl acetate, cis-	18	1334.4	19.5	1333		1310–1366	
Citronellyl acetate	86	1335.6	4.8	1335	1333–1337	1331–1344	
Bicycloelemene	9	1336.2	3.6	1336		1330–1341	
Eugenol	175	1339.6	16.1	1335	1327–1347	1323–1372	
δ-Elemene	109	1340.3	16.1	1337	1331–1343	1322–1381	
2-Undecenal, (E)-	16	1341.4	3.2	1340.5		1337–1347	
Piperitenone oxide	6	1342.3	15.4			1326–1368	
Thymol acetate	13	1342.7	7.3	1345		1330–1351	
Neryl acetate	112	1343.8	6.8	1343	1341–1345	1336–1353	
α-Longipinene	16	1350.6	12.2	1354.5		1327–1365	(d)
α-Cubebene	169	1352.2	11.7	1351	1345–1359	1334–1379	(d)
Carvacrol acetate	7	1354.4	9.2	1353		1344–1367	
1-Undecanol	20	1357.9	4.1	1357	1356–1361	1350–1365	1357 (Ref. 40)
Vanillin	54	1358.0	16.3	1350	1346–1367	1340–1392	
Geranyl acetate	167	1361.4	6.7	1361	1358–1363	1355–1370	
4,5-Epoxy-2-decenal, (E)-	1						1362 (Ref. 48)
Methyl cinnamate, trans-	10	1362.4	14.2	1364		1343–1380	
β-Damascenone, (E)-	61	1363.4	7.8	1361	1359–1368	1354–1375	
Decanoic acid	33	1363.5	13.1	1362	1354–1371	1346–1388	
Cyclosativene	10	1368.4	6.1	1368		1345–1406	(d)
Jasmone, (Z)-	26	1368.9	7.1	1368	1363–1376	1359–1379	
α-Ylangene	70	1370.0	9.7	1371	1364–1376	1353–1385	(d)
Longicyclene	8	1371.1	5.8	1370.5		1362–1378	
α-Copaene	318	1375.5	9.6	1375	1370–1380	1360–1392	
Methyl eugenol	75	1376.1	11.2	1373	1369–1378	1364–1402	
Daucene	10	1376.8	4.8	1379.5		1370–1382	
Isoitalicene	6	1378.0	2.5	1379		1374–1381	
Ethyl decanoate	52	1380.0	3.7	1379	1378–1382	1376–1387	
β-Bourbonene	159	1381.7	9.6	1381	1376–1386	1366–1400	
β-Cubebene	86	1383.5	7.7	1385	1380–1389	1370–1394	
β-Elemene	245	1388.0	12.4	1388	1384–1391	1372–1403	
α-Isocomene	11	1388.1	7.9			1377–1405	(d)
Dodecanal	69	1389.2	6.8	1388	1387–1392	1376–1401	
Decyl acetate	31	1392.3	3.4	1393	1390–1394	1387–1398	
Cyperene	22	1398.7	8.1	1398	1394–1404	1387–1409	(d)
Longifolene	39	1404.0	14.2	1400	1396–1409	1387–1433	
α-Gurjunene	75	1405.6	9.4	1406	1400–1411	1390–1422	
Italicene	7	1406.9	4.5	1407		1400–1415	(d)
2,5-Dimethoxy-p-cymene	5					1372–1422	
Caryophyllene, (Z)-	30	1407.7	14.1	1405	1396–1419	1384–1430	
α-Bergamotene, cis-	28	1410.3	9.4	1413	1406–1416	1395–1424	
α-Cedrene	56	1410.9	14.8	1411	1399–1416	1389–1436	(d)
α-Ionone, (E)-	36	1411.2	7.7	1411.5	1405–1416	1400–1422	
α-Santalene	18	1415.9	10.2	1412		1405–1435	
β-Ylangene	5	1416.3	7.2			1405–1425	
β-Cedrene	24	1417.7	8.2	1421	1409–1424	1401–1427	(d)
Caryophyllene, (E)-	563	1419.3	11.7	1419	1413–1424	1400–1442	
γ-Decalactone	23	1426.9	9.3	1425	1420–1430	1416–1447	

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TABLE 3. Retention indices of essential oil components for dimethylsilicone stationary phase—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
β-Copaene	42	1427.3	12.5	1426	1418–1438	1408–1446	
β-Gurjunene	71	1430.4	11.3	1430	1426–1435	1409–1448	(d)
Neryl propanoate	8	1430.6	2.9			1428–1436	
α-Bergamotene, trans-	86	1431.1	6.5	1432	1429–1435	1417–1440	
Geranylacetone	58	1431.1	7.9	1429	1427–1431	1422–1453	
Thujopsene, cis-	10	1433.9	9.4	1430		1425–1451	(d)
Aromadendrene	104	1439.0	13.7	1440	1429–1446	1413–1463	(d)
α-Guaiene	34	1442.4	10.4	1442	1436–1452	1427–1455	(d)
β-Farnesene, cis-	45	1443.7	9.5	1446	1440–1449	1428–1458	(d)
2-Dodecenal, (E)-	10	1444.3	2.9	1445		1439–1449	
α-Himachalene	13	1444.8	4.1	1443		1438–1451	
δ-Decalactone	15	1448.0	7.9	1447		1437–1463	
β-Humulene	6	1448.0	6.2	1448.5		1439–1454	(d)
β-Farnesene, (E)-	186	1449.3	9.6	1448	1445–1452	1438–1466	
α-Humulene	398	1449.3	10.8	1451	1443–1455	1430–1466	
γ-Elemene	45	1449.3	29.5	1438	1427–1482	1418–1499	
Geranyl propanoate	17	1449.3	3.8	1448		1444–1461	
Muurola-4 (14),5-diene, cis-	5	1449.8	7.2	1454		1438–1455	
α-Patchoulene	6	1451.3	8.6	1450.6		1443–1464	
β-Santalene	11	1453.0	6.6	1450		1445–1467	
Undecanoic acid	3	1458.0	12.1			1445–1469	1445 (Ref. 49)
Alloaromadendrene	147	1459.1	9.4	1460	1453–1464	1445–1477	
1-Dodecanol	42	1459.8	8.6	1460	1456–1465	1443–1474	
β-Acoradiene	6	1461.8	7.8	1461		1454–1475	
Phenylethyl 3-methylbutanoate	13	1464.9	9.3	1465		1448–1483	
β-Ionone, (E)-	91	1466.2	6.8	1466	1462–1470	1454–1480	
α-Amorphene	23	1466.2	14.6	1470	1451–1475	1449–1491	
γ-Gurjunene	27	1467.3	10.9	1469	1461–1475	1447–1484	
β-Chamigrene	14	1470.1	8.7	1474		1450–1479	
γ-Himachalene	5	1471.2	8.1	1468		1461–1480	
Ar-Curcumene	91	1471.4	10.2	1472	1465–1475	1453–1489	
γ-Curcumene	20	1472.7	6.0	1473	1471–1474	1460–1481	
γ-Muurolene	146	1473.0	10.8	1472	1467–1479	1455–1494	
Germacrene D	304	1475.9	9.8	1476	1471–1481	1458–1491	
β-guaiene, cis-	18	1478.6	11.7	1482		1458–1490	
2-Tridecanone	38	1478.8	6.6	1477	1475–1481	1470–1492	
α-Farnesene, (Z,E)-	9	1480.6	6.2	1480		1470–1492	
β-Selinene	140	1480.7	9.9	1482	1476–1486	1463–1498	
α-Zingiberene	42	1482.9	11.4	1487	1474–1490	1463–1494	
Valencene	60	1483.0	10.9	1484	1477–1490	1461–1498	
Eugenol acetate	11	1484.5	5.3	1485		1474–1493	
Viridiflorene	38	1488.9	8.4	1492	1484–1494	1472–1499	
Cubebol, epi-	11	1489.0	4.6	1488		1482–1498	
α-Selinene	107	1489.5	10.7	1490	1484–1495	1470–1509	
Bicyclogermacrene	160	1489.8	8.6	1491	1486–1495	1474–1501	
Germacrene A	19	1490.6	11.8	1490		1476–1509	
α-Muurolene	151	1491.0	8.0	1493	1486–1496	1477–1502	
Tridecanal	32	1491.1	4.6	1490	1488–1494	1483–1499	
Geranyl isobutanoate	6	1491.3	3.1	1492		1487–1495	
β-Guaiene, trans-	6	1492.0	14.0			1470–1503	(h)
Myristicin	19	1494.4	12.2	1493	1487–1450	1477–1517	
α-Bisabolene, (Z)-	10	1496.2	2.9	1496		1496–1501	
α-Farnesene, (E,E)-	120	1496.3	8.1	1495	1492–1500	1484–1509	
β-Bisabolene	175	1499.9	7.4	1500	1495–1505	1485–1511	
α-Bulnesene	27	1500.6	9.8	1502	1492–1503	1489–1517	
β-Himachalene	11	1500.8	7.1	1499		1494–1517	(d)
β-Curcumene	15	1503.0	5.2	1502		1493–1513	

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TABLE 3. Retention indices of essential oil components for dimethylsilicone stationary phase—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
Cuparene	20	1504.8	8.7	1504	1498–1510	1490–1519	
Cubebol	21	1504.9	9.0	1507.5	1499–1512	1487–1515	
γ-Cadinene	202	1505.7	10.3	1507	1499–1512	1490–1521	
Citronellyl butanoate	8	1506.2	3.3	1506		1503–1511	
α-Selinene, 7-epi-	7	1507.9	12.6	1508		1492–1527	
Calamenene, cis-	90	1509.6	10.6	1510	1503–1517	1492–1528	
γ-Bisabolene, (Z)-	13	1511.7	3.1	1512		1505–1516	
Calamenene, trans-	32	1512.8	6.3	1512.5	1510–1515	1505–1524	
β-Sesquiphellandrene	54	1513.2	6.9	1514	1510–1518	1500–1523	
δ-Cadinene	346	1513.9	8.4	1515	1509–1519	1498–1526	
Elemicin	33	1521.4	6.3	1521	1516–1526	1512–1531	
Cadina-1(2),4-diene, cis	34	1523.9	8.3	1525	1518–1529	1511–1536	
Nerolidol, (Z)-	41	1524.4	11.1	1524	1516–1533	1509–1543	
γ-Bisabolene, (E)-	10	1525.6	4.4	1525.5		1520–1532	
α-Cadinene	54	1526.6	10.2	1528	1521–1532	1506–1542	
α-Calacorene	63	1530.4	9.5	1531	1525–1538	1514–1543	
α-Bisabolene, (E)-	10	1533.6	4.2	1533		1527–1543	
Sesquisabinene hydrate, cis-	8	1534.8	9.2			1521–1540	
Germacrene B	90	1535.1	25.7	1544	1528–1554	1483–1562	
Elemol	90	1536.2	10.9	1535	1530–1543	1518–1555	
Geranyl butanoate	29	1537.1	8.7	1534	1532–1540	1529–1555	
β-Elemol	11	1537.2	3.4	1537		1530–1543	
Selina-3,7(11)-diene	10	1537.9	4.1	1540		1530–1542	
β-Calacorene	21	1547.1	8.4	1548	1547–1552	1527–1555	
3-Hexenyl benzoate, (Z)-	24	1549.8	7.7	1549	1543–1554	1540–1563	
Nerolidol, (E)-	154	1550.1	8.6	1549	1546–1553	1538–1565	
Hexyl benzoate	24	1554.3	6.3	1552	1550–1559	1545–1565	
β-Phenylethyl tiglate	11	1556.8	3.6	1555		1554–1566	
Caryophyllenyl alcohol	9	1560.0	5.9	1559		1551–1572	
Dendrolasin	3	1561.3	3.5			1558–1565	
Palustrol	16	1562.1	7.8	1562.5		1548–1579	
Dodecanoic acid	31	1563.7	18.8	1558	1550–1574	1544–1601	
Spathulenol	192	1566.4	10.4	1568	1560–1573	1549–1580	
Globulol, epi-	8					1540–1597	(h)
Germacrene-D-4-ol	20	1568.3	8.4	1570	1560–1575	1553–1579	
Caryophyllene oxide	317	1570.0	11.6	1573	1565–1578	1549–1587	
Gleenol	6	1574.2	2.3	1574		1572–1578	
β-Copaen-4α-ol	7	1577.9	4.7	1575		1572–1584	
Ethyl dodecanoate	38	1578.2	5.5	1578	1577–1581	1566–1588	
Globulol	89	1578.9	11.3	1579	1570–1587	1561–1595	
Viridiflorol	79	1579.9	11.2	1580	1572–1587	1561–1598	
Ledol	56	1582.5	17.2	1585.5	1578–1597	1545–1601	(d)
Sesquisabinene hydrate, trans-	9	1584.4	10.7	1580		1573–1602	
Salvial-4(14)-en-1-one	11	1584.7	6.5	1584		1576–1593	
Geranyl isovalerate	17	1587.5	9.2	1585		1573–1605	
Guaiol	34	1588.9	7.9	1588.5	1584–1594	1576–1603	
α-Humulene oxide	19	1590.7	12.9	1588		1570–1612	
Longiborneol	5	1592.2	9.4	1592		1579–1603	(d)
Carotol	6	1592.8	5.0	1594		1587–1600	
β-Oplopenone	12	1592.9	6.0	1592		1586–1607	
Tetradecanal	39	1594.7	8.6	1592	1591–1596	1585–1614	
Dill apiole	7	1596.3	9.9	1595		1582–1613	
Humulene epoxide II	49	1597.1	9.2	1598	1596–1601	1575–1609	
Cedrol	24	1597.1	13.3	1598	1584–1609	1576–1615	(d)
Cubenol, 1,10-di-epi-	14	1605.5	7.5	1608		1590–1614	
γ-Eudesmol, 10-epi-	28	1607.9	8.3	1613	1598–1613	1595–1617	
1-Cubenol, epi-	40	1614.0	10.1	1617	1607–1621	1595–1628	

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TABLE 3. Retention indices of essential oil components for dimethylsilicone stationary phase—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
γ-Eudesmol	54	1616.5	9.6	1618	1607–1625	1602–1630	
Cubenol	75	1619.9	13.9	1618	1610–1632	1600–1644	
α-Acorenol	8	1620.3	8.8	1621		1605–1630	
Caryophylla-4(12),8(13)-dien-5α-ol	8	1623.9	2.4	1623		1622–1628	
Isospathulenol	5	1625.6	4.2	1626		1619–1630	
α-Cadinol, epi-	146	1626.4	9.8	1627	1617–1633	1612–1642	
α-Muurolol	86	1626.6	14.6	1626	1618–1638	1605–1650	
α-Muurolol, epi-	110	1631.2	10.8	1631.5	1626–1637	1610–1650	
β-Eudesmol	114	1633.7	14.3	1535.5	1627–1643	1611–1655	
Intermedeol	10	1636.1	11.2	1629.5		1626–1653	
α-Cadinol	171	1640.2	12.3	1641	1631–1647	1619–1662	
Selin-11-en-4α-ol	13	1641.1	7.1	1640		1632–1656	
α-Eudesmol	68	1641.1	13.2	1643	1634–1647	1619–1668	
Himachalol	1						1648 (Ref. 49)
Patchouli alcohol	8	1653.2	14.1	1657.5		1625–1667	
Bulnesol	15	1653.3	4.8	1652		1645–1664	
Valeranone	10	1654.2	14.6	1660		1633–1668	
Cadalene	30	1654.9	10.6	1654	1646–1662	1641–1673	
Caryophyllenol II	1						1655 (Ref. 50)
β-Bisabolol	25	1658.6	9.4	1658	1653–1664	1644–1674	
Tridecanoic acid	7	1659.1	9.4	1660		1645–1668	
1-Tetradecanol	15	1663.1	10.9	1664		1647–1680	
α-Bisabolol	78	1668.4	9.9	1668.5	1663–1674	1649–1686	
β-Sinensal	19	1669.6	4.6	1671		1658–1675	
Geranyl tiglate	10	1673.7	7.0	1675		1659–1688	
α-Bisabolol, epi-	18	1674.3	12.9	1676.5		1651–1690	
Eudesma-4(15),7-dien-1β-ol	6	1675.8	5.0	1676.5		1670–1681	
2-Pentadecanone	29	1680.8	6.2	1681	1678–1684	1671–1690	
Eudesm-7(11)-en-4-ol	9	1681.6	7.5	1680		1674–1700	
Farnesol, (2Z,6Z)-	12	1686.9	7.1	1687		1678–1699	(i)
Farnesol, (2E,6Z)-	6	1691.3	2.0	1692		1688–1693	(i)
Pentadecanal	24	1695.5	6.6	1694	1692–1697	1690–1712	
Farnesol, (2Z,6E)-	55	1704.7	10.9	1704	1699–1712	1683–1723	(i)
Methyl tetradecanoate	33	1709.4	4.0	1708	1707–1713	1705–1716	
Farnesol, (2E,6E)-	14	1709.6	14.7	1709		1693–1732	(i), 1708 (Ref. 51)
Chamazulene	11	1710.0	5.8	1712		1700–1716	
α-Sinensal	10	1727.5	6.3	1726		1720–1742	
Benzyl benzoate	76	1733.5	19.3	1730	1722–1741	1706–1774	
Tetradecanoic acid	51	1753.3	14.3	1750	1743–1763	1732–1780	
Nootkatone	19	1776.5	16.8	1775		1746–1802	
Ethyl tetradecanoate	32	1778.0	4.6	1778	1777–1780	1770–1785	
Hexadecanal	29	1797.1	9.1	1795	1794–1796	1784–1814	
Farnesyl acetate, (2E,6E)-	15	1818.1	5.4	1816		1810–1828	
Hexahydrofarnesylacetone	22	1832.9	10.8	1833	1824–1837	1817–1850	
Benzyl salicylate	18	1837.2	14.5	1835		1815–1860	
Pentadecanoic acid	22	1853.8	11.0	1852	1844–1866	1840–1869	
1-Hexadecanol	35	1861.6	8.1	1862	1856–1866	1851–1876	
2-Heptadecanone	19	1883.1	5.8	1883		1871–1891	
Methyl hexadecanoate	69	1909.4	4.1	1909	1907–1911	1902–1917	
Farnesyl acetone, (5E,9E)	5	1914.2	3.1	1915		1911–1918	
Hexadec-9-enoic acid, (Z)-	13	1935.2	5.0	1936		1929–1945	
Isophytol	11	1938.5	11.6	1940		1920–1956	
Hexadecanoic acid	90	1955.4	13.6	1953.5	1943–1966	1937–1979	
Ethyl hexadecanoate	40	1978.1	4.1	1978	1977–1980	1969–1985	
Manoyl oxide	18	1990.4	6.9	1991		1977–2000	(d)
Manool, 13-epi-	6	2008.3	6.2	2008		1999–2016	2006 (Ref. 45)
Abietatriene	17	2032.8	13.3	2034		2013–2052	

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TABLE 3. Retention indices of essential oil components for dimethylsilicone stationary phase—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
Manool	6	2047.5	22.2	2047		2026–2087	
1-Octadecanol	14	2060.0	8.5	2061		2040–2070	
Abietadiene	6	2061.8	11.1	2064		2044–2073	
Methyl linoleate	16	2078.8	12.3	2076		2061–2100	
Methyl oleate	28	2081.3	8.1	2080	2076–2084	2072–2100	
Phytol	35	2099.1	14.5	2101	2091–2106	2074–2121	
Linoleic acid	9	2105.0	6.9	2107		2095–2113	2100–2105 (Ref. 40)
Methyl octadecanoate	48	2112.1	9.8	2109	2107–2114	2101–2132	
Oleic acid	2					2091–2113	
Ethyl linoleate	10	2150.5	13.4	2143		2139–2177	
Octadecanoic acid	16	2158.7	19.8			2137–2193	2140–2142 (Ref. 40)

Comments: (a) Number of data records. (b) Confidence interval estimates were based on the number of available data records. The range of available RI values was used for compounds with less than 20 data-records instead of estimation of confidence intervals. (c) Retention indices[7] are provided as linear retention indices. Previous editions[7] listed retention indices determined using logarithmic times. RI data[40] were rounded to integer values. Shown RI data ranges correspond to RI measurements at two temperature programs.[40] (d) Observed RI values were close for dimethylsilicone and 5% phenylmethylsilicone stationary phases, or the retention index was higher for dimethylsilicone phase. (e) The correct identification of o-, m-, and p-cymenes presents certain difficulties. Inconsistencies in available literature retention data and elution order for these isomers were discussed by Collin *et al*.[41] Note that most of the researchers registered only one of the three isomers. The most frequently observed isomer is p-cymene. Data presented in Table 1 are largely based on the results of Collin *et al*.,[41] and Romanenko *et al*.[42] Note that the observed elution order is in agreement with the correlation between boiling points and elution order of isomers. It is known that for isomers of the same homologous series the elution order on nonpolar stationary phases corresponds to the order of their boiling points. Thus the first eluted isomer should be meta-, and the last—ortho-isomer (m-cymene (448.3 K) < p-cymene (450.3 K) < o-cymene (451.3 K) (Ref. 43)). (f) Available literature data represent a mix of data for cis- and trans-isomers as a result of the use of different naming conventions. The name was provided in accord with IUPAC nomenclature (OH vs. IPP). Data separation was performed based on the elution order. (g) Available data possibly represent a mix of RI values for different isomers. (h) Two (or more) separate data clusters or a large data spread were observed. (i) There are 4 isomers of farnesol. Most of the available RI measurements (elution order) correspond to the data provided in the earlier editions of Adams.[7] 2007 edition contains the re-identification of these isomers. The re-identification is consistent with the results,[92–97] where detailed analysis of farnesol isomers was conducted. We adopted these results for the reassignment of calculated retention indices.

TABLE 4. Retention indices of essential oil components for dimethylsilicone stationary phase with 5% phenyl groups

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
2,3-Butanedione	112	596.6	11.1	595	590–613	581–605	
Ethyl acetate	82	611.2	11.3	612.5	607–615	588–628	
Acetic acid	76	622.3	26.2	610	601–645	591–667	(d)
Isobutanol	56	630.5	12.8	628	622–637	615–655	650 (Ref. 7)
3-Methylbutanal	172	651.6	11.5	652	649–658	629–669	
Butanal, 2-methyl-	121	660.2	12.9	662	653–668	635–680	
1-Butanol	48	660.2	10.1	660.5	653–667.3	644–677	
1-Penten-3-ol	41	690.1	15.4	685	681–689	673–722	
Pentanal	105	700.3	11.2	699	696–704	683–722	
2-Ethylfuran	48	704.6	8.1	703	701–707	691–719	
Acetoin	73	713.7	12.6	714	711–720	697–733	
3-Methyl-1-butanol	125	737.5	10.7	736	732–741	726–758	
Butan-1-ol, 2-methyl-	81	740.8	8.8	740	734–744	730–756	
1-Pentanol	101	765.5	7.1	765	763–768	756–779	
2-Pentenol, (Z)-	14	771.2	5.8	769		767–783	
2-Buten-1-ol, 3-methyl-	30	774.6	8.1	776.5	770–779	759–788	
Ethyl butanoate	131	799.0	8.7	802	798–804	778–807	
3-Hexenal, (Z)-	53	799.5	5.7	800	798–801	789–807	
Hexanal	343	799.9	7.7	800	799–803	782–810	
Butanoic acid	81	808.3	19.6	815	790–821	779–840	763 (Ref. 7)
Furfural	124	834.6	11.1	834	830–840	814–851	
3-Hexen-1-ol, (E)-	55	852.8	8.8	852	852–857	837–863	844 (Ref. 7)
2-Hexenal, (E)-	187	853.0	9.2	854	851–856	837–865	

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TABLE 4. Retention indices of essential oil components for dimethylsilicone stationary phase with 5% phenyl groups—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
Ethyl isovalerate	60	853.1	6.6	854	851–856	842–864	
3-Hexen-1-ol, (Z)-	111	856.6	7.2	857	853–860	844–868	
Isovaleric acid	93	860.4	19.9	868	841–875	832–889	827 (Ref. 7); 858–868 (Ref. 40)
Butanoic acid, 2-methyl-	71	861.9	17.8	863	847–875	836–890	832 (Ref. 7)
Furfuryl alcohol	45	862.6	10.6	863	853–867	850–881	
2-Hexen-1-ol, (E)-	48	864.5	10.6	862	857–869	852–887	
1-Hexanol	148	869.7	7.9	868	866–874	859–885	
Isopentyl acetate	79	875.0	7.1	876	875–878	860–883	869 (Ref. 7)
Styrene	75	890.5	13.2	893	880–897	870–915	
2-Heptanone	143	891.7	4.6	891	889–893	884–900	
2-Heptanol	40	899.4	8.6	900	898–904	881–909	
Ethyl pentanoate	33	901.2	2.6	901	900–902	898–906	
Heptanal	203	902.0	5.5	901	899–904	894–913	
Santolina triene	25	907.4	4.5	908	905–909	900–914	
Methional	172	907.5	6.2	907	904–910	900–920	
2-Acetylfuran	40	912.4	9.1	910	907–917	902–928	
2,4-Hexadienal-, (2E,4E)-	22	913.2	5.1	912	909–916	908–924	
Tricyclene	179	923.2	7.0	925	921–927	906–931	
Methyl hexanoate	51	924.1	7.9	925	922–929	909–934	
α-Thujene	384	927.8	6.8	930	926–931	910–935	
α-Pinene	765	936.1	8.0	937	933–939	921–944	
α-Fenchene	48	949.4	6.5	951	948–953	939–957	
Camphene	480	950.3	7.0	952	948–954	936–959	
Thuja-2,4(10)-diene	45	955.6	3.8	957	955–958	947–959	
2-Heptenal, (E)-	46	960.5	8.3	959.5	956–964	952–978	947 (Ref. 7)
Benzaldehyde	304	962.7	10.4	962	959–967	947–982	
Verbenene	44	963.3	9.5	967	953–968	948–976	
Furfural, 5-methyl-	58	967.3	9.9	965.5	961–973	953–987	
1-Heptanol	48	968.6	11.2	970	968–974	945–980	959 (Ref. 7)
Dimethyl trisulfide	127	971.7	10.3	970	965–979	954–989	
Sabinene	472	973.0	7.0	975	971–976	961–981	
β-Pinene	643	977.7	7.1	979	975–980	964–988	
1-Octen-3-one	148	978.0	5.2	979	976–980	968–986	
1-Octen-3-ol	268	980.0	8.1	980	978–983	967–991	
Phenol	49	983.3	7.8	981	978–987	974–997	
3-Octanone	76	984.5	6.4	986	982–988	971–994	
6-Methyl-5-hepten-2-one	163	985.9	5.7	986	984–988	977–995	
Myrcene	655	989.2	6.2	991	988–992	980–995	
Dehydro-1,8-cineole	39	989.8	9.1	991	988–993	971–1005	
5-Hepten-2-ol, 6-methyl-	11	991.8	7.7	993		979–1003	
2-Pentylfuran	112	991.9	5.7	993	990–995	978–999	
3-Octanol	98	993.2	6.7	993	991–995	981–1005	
Yomogi alcohol	15	996.3	3.8	998		989–1000	
Hexanoic acid	92	996.4	20.5	993	981–1018	969–1026	
Ethyl hexanoate	130	999.6	4.0	1000	997–1002	994–1005	
Octanal	279	1002.8	6.5	1003	1001–1005	993–1012	
δ-2-Carene	51	1003.3	7.3	1001	1000–1004	994–1020	
3-Hexenyl acetate, (Z)-	66	1004.0	7.7	1005	999–1007	988–1016	
α-Phellandrene	395	1004.1	6.8	1004	1002–1006	995–1013	
2-Methylpropyl 3-methylbutanoate	8	1008.5	5.6	1006		1003–1018	
Hexyl acetate	81	1010.4	6.4	1011	1008–1015	999–1020	
3-Carene	267	1011.3	6.4	1011	1008–1013	1002–1025	
2,4-Heptadienal, (2E,4E)-	70	1011.5	7.4	1012	1009–1017	996–1019	1005 (Ref. 7)
2-Hexen-1-ol, acetate, (E)-	10	1011.5	9.7	1017		994–1020	
1,4-Cineole	16	1016.8	5.9	1016		1008–1033	
α-Terpinene	416	1017.1	7.3	1017	1015–1019	1007–1026	

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TABLE 4. Retention indices of essential oil components for dimethylsilicone stationary phase with 5% phenyl groups—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
m-Cymene	27	1022.0				997–1037	(e); average of data (Refs. 41 and 42)
p-Methyl anisole	10	1023.8	5.6	1024		1018–1036	1015 (Ref. 7)
p-Cymene	627	1024.3	7.0	1025	1022–1027	1011–1033	(e); 1026 (Ref. 41); 1024 (Ref. 42)
Limonene	753	1029.5	6.9	1030	1027–1032	1019–1039	
β-Phellandrene	222	1030.0	9.6	1030	1029–1033	1011–1043	
1-Hexanol, 2-ethyl-	50	1030.6	7.1	1030	1028–1034	1016–1042	
1,8-Cineole	444	1031.8	6.9	1032	1030–1034	1021–1044	
Benzyl alcohol	118	1036.9	8.0	1035	1032–1041	1026–1052	
β-Ocimene, (Z)-	328	1037.8	6.7	1038	1036–1040	1028–1047	
o-Cymene	85	1041.0				1001–1076	(e); average of data (Refs. 41 and 42)
Benzeneacetaldehyde	281	1045.9	9.7	1045	1042–1051	1032–1063	
Salicylaldehyde	11	1046.5	7.6	1041		1040–1063	
β-Ocimene, (E)-	420	1047.7	6.2	1049	1046–1051	1038–1056	
γ-Terpinene	575	1059.7	7.5	1060	1057–1062	1049–1069	
2-Octenal, (E)-	93	1060.2	6.8	1060	1057–1063	1046–1072	1049 (Ref. 7)
Artemisia ketone	19	1062.0	4.2	1062		1050–1071	
Sabinene hydrate, cis-	205	1066.5	7.3	1068	1065–1070	1052–1074	(f)
2-Octen-1-ol, (E)-	14	1066.8	4.5	1069		1059–1071	1049 (Ref. 7)
Acetophenone	80	1067.4	7.4	1066	1063–1072	1056–1080	
1-Octanol	163	1071.5	6.2	1071	1068–1074	1063–1083	
Furaneol	77	1072.3	15.8	1070	1061–1080	1051–1100	
Linalool oxide, (furanoid), cis-	142	1075.1	8.8	1074	1071–1078	1061–1090	
p-Cresol	72	1077.4	9.9	1077	1074–1083	1058–1093	
Heptanoic acid	21	1080.1	10.7	1078	1072–1086	1067–1098	(d)
Artemisia alcohol	25	1083.1	4.9	1084	1083–1084	1072–1092	
Linalool oxide, (furanoid), trans-	123	1083.3	8.6	1087	1074–1088	1070–1097	
Terpinolene	476	1086.9	7.7	1088	1086–1089	1074–1097	
Fenchone	40	1087.6	5.6	1087	1087–1090	1078–1096	
p-Cymenene	90	1087.9	9.5	1090	1087–1091	1066–1098	
o-Guaiacol	89	1092.1	6.7	1090	1087–1095	1086–1106	
2-Nonanone	104	1092.5	4.2	1093	1091–1094	1083–1099	
Methyl benzoate	60	1094.2	7.3	1094	1091–1097	1080–1106	
α-Pinene oxide	22	1097.0	5.7	1095	1095–1100	1090–1105	
Sabinene hydrate, trans-	118	1098.1	8.2	1097	1096–1101	1084–1115	(f)
2-Nonanol	8	1098.6	13.6	1098		1076–1120	
Perillene	15	1098.6	4.8	1100		1083–1102	(d)
Linalool	716	1099.0	6.8	1099	1097–1102	1088–1109	
Nonanal	436	1103.3	6.7	1104	1102–1106	1093–1118	
Isopentyl isovalerate	33	1103.6	4.1	1103	1103–1105	1094–1110	
Thujone, cis-	87	1105.1	6.1	1102	1102–1107	1099–1117	
Hotrienol	12	1106.8	5.1	1106.5		1101–1114	
1-Octen-3-yl acetate	26	1110.3	6.1	1111	1110–1114	1097–1119	
1,3,8-p-Menthatriene	36	1111.7	4.2	1112	1110–1113	1107–1117	
Rose oxide, cis-	27	1112.5	6.9	1112	1110–1113	1103–1126	
Myrcenol	7	1113.1	15.3	1117		1091–1137	
2,4-Octadienal-, (2E,4E)-	16	1113.9	3.5	1115		1110–1124	1102 (Ref. 7)
Thujone, trans-	88	1114.5	5.1	1114	1114–1116	1106–1124	
2-Phenylethyl alcohol	208	1114.9	14.9	1116	1110–1120	1100–1129	
Fenchol, endo-	50	1115.1	6.3	1114	1112–1117	1110–1125	
Pinene hydrate, trans-	16	1121.2	4.1	1121		1114–1127	
p-Menth-2-en-1-ol, cis-	106	1123.1	7.1	1122	1121–1126	1115–1138	
α-Campholenal	138	1124.1	8.4	1125	1124–1127	1106–1134	
Chrysanthenone	26	1124.5	3.2	1123.5	1123–1126	1120–1131	
Isophorone	21	1127.2	10.4	1122	1118–1137	1117–1144	
Tagetone, (E)-	7	1127.3	7.5	1124		1120–1139	1139 (Ref. 7); 1128 (Ref. 52)

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TABLE 4. Retention indices of essential oil components for dimethylsilicone stationary phase with 5% phenyl groups—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
p-Mentha-2,8-dien-1-ol, trans-	11	1127.5	6.9	1123		1122–1142	
Methyl octanoate	35	1127.5	4.9	1126	1125–1128	1121–1138	
Rose oxide, trans-	11	1128.4	9.4	1127		1115–1149	
allo-Ocimene	54	1129.9	4.1	1130	1128–1132	1124–1135	
p-Mentha-2,8-dien-1-ol, cis-	13	1131.4	9.1	1134		1119–1149	
Limonene oxide, cis-	41	1134.0	6.2	1134	1131–1138	1122–1144	
Nopinone	15	1135.5	5.3	1137		1120–1145	
Terpine-1-ol	27	1136.1	5.6	1136	1134–1140	1127–1145	
p-Menth-2-en-1-ol, trans-	76	1136.7	11.6	1140	1138–1143	1112–1147	
Limonene oxide, trans-	32	1137.5	6.9	1138	1134–1142	1126–1149	
Sabinol, trans-	24	1139.2	3.1	1140	1139–1140	1134–1142	
Pinocarveol, trans-	186	1140.0	11.5	1139	1136–1141	1124–1163	
Sabinol, cis-	12	1142.4	2.9	1143		1137–1149	
Camphor	301	1143.4	7.9	1144	1142–1146	1127–1155	
β-Terpineol, cis-	8	1143.9	5.2	1145		1132–1150	
Verbenol, trans-	80	1144.2	2.8	1144	1143–1146	1139–1148	
Verbenol, cis-	71	1144.4	8.5	1142	1140–1145	1134–1165	
Phenylacetonitrile	19	1146.5	8.7	1144		1135–1163	
2-Nonenal, (Z)-	55	1146.8	3.8	1148	1146–1149	1142–1151	
4-Ketoisophorone	14	1147.4	9.1	1142		1139–1169	
Veratrole	21	1148.1	4.6	1148	1146–1152	1140–1154	
Camphene hydrate	33	1148.7	3.8	1148	1148–1150	1144–1155	
Tagetone, (Z)-	5	1149.4	4.1	1149		1144–1155	1148 (Ref. 7); 1136 (Ref. 52)
Menthone	49	1150.5	14.2	1154	1144–1156	1125–1174	
Citronellal	77	1153.7	5.8	1153	1152–1156	1144–1162	
2,6-Nonadienal, (2E,6Z)-	108	1154.7	4.5	1155	1152–1158	1148–1162	
Nerol oxide	12	1154.7	8.0	1154		1146–1172	
Sabina ketone	24	1155.7	4.5	1156	1154–1158	1147–1162	
Isoborneol	52	1158.2	7.9	1156.5	1155–1162	1146–1173	
Isomenthone	39	1159.1	16.2	1164	1150–1169	1132–1183	
Pinocarvone	141	1160.6	6.4	1162	1160–1164	1144–1167	
Pinocamphone, trans	38	1162.0	6.3	1160	1159–1163	1155–1175	
2-Nonenal, (E)-	169	1162.2	6.2	1161	1158–1165	1154–1173	
Chrysanthenol, cis-	23	1162.9	2.2	1162	1162–1164	1160–1168	
Menthofuran	13	1164.2	9.1	1164		1142–1183	
δ-Terpineol	20	1164.5	5.7	1166	1163–1167	1153–1171	
Benzyl acetate	46	1165.6	6.3	1164	1162–1169	1160–1178	
Borneol	322	1166.2	7.9	1166	1164–1169	1152–1177	
p-Mentha-1,5-dien-8-ol	68	1166.6	7.2	1167	1164–1170	1155–1179	
neo-Menthol	7	1167.4	5.1	1166		1161–1176	
1,4-Dimethoxybenzene	18	1167.6	13.7	1165		1143–1192	
Lavandulol	16	1168.2	6.3	1168		1155–1185	
Linalool oxide (pyranoid), trans-	6	1171.0	5.3	1172		1162–1178	
Ethyl benzoate	51	1171.3	6.5	1171	1170–1175	1160–1182	
Umbellulone	21	1171.4	5.6	1171	1169–1171	1165–1184	
Pinocamphone, cis	34	1172.8	4.7	1173	1172–1175	1162–1180	
1-Nonanol	38	1173.4	5.8	1172	1171–1175	1167–1184	1165 (Ref. 7)
Isopulegone, trans-	8	1176.6	15.6	1176		1155–1199	
Terpinen-4-ol	593	1177.1	9.0	1177	1175–1179	1165–1189	
Limonen-4-ol	6	1177.3	7.6	1176.5		1167–1189	
Menthol	46	1177.3	8.6	1174	1172–1182	1169–1194	
1(7),8-p-Menthadien-2-ol, trans-	2	1180.5				1176–1185	1187 (Ref. 7)
Octanoic acid	66	1182.0	10.8	1180	1176–1189	1164–1200	
p-Methylacetophenone	28	1182.7	5.9	1182.5	1180–1187	1174–1191	
Cryptone	28	1183.6	7.8	1184	1178–1187	1172–1199	
p-Cymen-8-ol	171	1183.9	4.5	1183	1183–1185	1178–1191	
3-Hexenyl butanoate, (Z)-	21	1184.7	3.8	1186	1184–1187	1178–1188	

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TABLE 4. Retention indices of essential oil components for dimethylsilicone stationary phase with 5% phenyl groups—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
Naphthalene	106	1186.2	12.4	1183	1179–1192	1170–1211	
α-Terpineol	624	1189.7	9.4	1189	1188–1192	1178–1203	
Hexyl butanoate	29	1191.5	4.0	1191	1191–1194	1184–1198	
Myrtenal	115	1192.0	9.8	1193	1190–1196	1171–1206	
p-Cresol, 2-methoxy-	19	1192.9	5.7	1192		1181–1207	
Methyl salicylate	95	1192.9	6.3	1192	1190–1194	1184–1208	
Myrtenol	159	1194.1	9.3	1194	1193–1197	1177–1206	
Dihydrocarveol	18	1194.5	7.8	1183		1181–1208	1192 (Ref. 7)
Piperitol, cis-	52	1194.7	8.3	1195	1193–1196	1180–1211	
Methyl chavicol	69	1195.8	5.2	1196	1195–1198	1184–1204	
Ethyl octanoate	94	1196.2	5.9	1196	1194–1200	1190–1205	
Dihydrocarvone, trans-	38	1201.4	4.7	1200	1199–1202	1196–1211	
Piperitol, trans-	69	1205.3	6.8	1207	1205–1208	1192–1214	
Decanal	301	1205.4	7.6	1205	1204–1208	1195–1217	
Verbenone	132	1206.2	11.4	1205	1204–1208	1190–1224	
Octanol acetate	46	1209.3	6.3	1210.5	1208–1213	1196–1219	
iso-Dihydrocarveol	11	1213.4	9.5	1213		1196–1227	
Cinnamaldehyde, cis-	6	1215.2	7.6			1200–1219	
2,4-Nonadienal, (2E,4E)-	88	1215.8	7.4	1216	1211–1219	1204–1230	
Carveol, trans-	156	1217.1	8.0	1217	1216–1219	1203–1231	
β-Cyclocitral	46	1218.3	6.9	1219.5	1216–1223	1205–1225	
Sabinene hydrate acetate, cis-	12	1218.7	7.3	1220		1213–1229	
Fenchyl acetate, endo-	21	1219.7	5.4	1220	1220–1221	1210–1223	
Bornyl formate	8	1222.6	7.7	1223		1206–1232	
Carveol, cis-	75	1226.7	7.6	1229	1222–1230	1214–1239	
Citronellol	129	1228.1	6.0	1228	1226–1231	1215–1237	
Nerol	125	1228.9	9.5	1228	1226–1230	1216–1250	
1(7),8-p-Menthadien-2-ol, cis-	2	1233.0				1231–1235	
Thymol, methyl ether	85	1234.3	3.9	1235	1233–1236	1229–1240	
Pulegone	64	1234.3	12.1	1237	1232–1239	1210–1253	
Hexyl 2-methyl butanoate	21	1236.3	4.3	1235	1234–1237	1233–1243	
Cumin aldehyde	94	1237.9	9.2	1239	1235–1242	1220–1253	
Carvone	181	1242.0	11.2	1242	1240–1245	1227–1265	
Neral	116	1242.1	9.6	1240	1237–1244	1231–1269	
Carvacrol, methyl ether	47	1243.0	4.3	1244	1243–1245	1234–1247	
Carvotanacetone	10	1245.3	6.4	1246		1230–1256	
p-Anisaldehyde	35	1251.8	8.9	1251	1247–1255	1239–1266	
Sabinene hydrate acetate, trans-	14	1253.4	7.7	1252		1243–1272	
Piperitone	91	1253.6	6.7	1252	1251–1255	1245–1266	
Chavicol	11	1253.9	5.3	1254		1248–1265	
Geraniol	247	1254.9	9.0	1255	1253–1258	1238–1269	
Linalool acetate	117	1255.2	8.9	1257	1251–1259	1238–1268	
2-Phenylethyl acetate	61	1258.8	7.1	1258	1256–1260	1245–1269	
Chrysanthenyl acetate, cis-	33	1261.8	3.3	1262	1261–1263	1255–1267	
2-Decenal, (E)-	91	1263.4	5.4	1263	1260–1266	1255–1276	
Geranial	142	1270.3	9.8	1270	1267–1273	1252–1291	
Cinnamaldehyde, trans-	20	1271.3	8.1	1270	1267–1274	1264–1287	
1-Decanol	32	1272.1	6.8	1272	1269–1274	1263–1286	
Perilla aldehyde	37	1273.4	10.7	1271	1270–1277	1257–1292	
Phellandral	13	1274.9	10.1	1273		1255–1298	
Nonanoic acid	46	1275.3	9.9	1275	1267–1280	1260–1293	1267 (Ref. 7)
Citronellyl formate	6	1276.7	3.9	1276		1271–1282	
Methyl 3-phenylpropionate	9	1278.6	16.8	1279		1248–1296	
Guaiacol, 4-ethyl-	31	1280.2	7.4	1282	1276–1286	1266–1288	
p-Anisyl alcohol	12	1282.3	7.5	1279		1273–1295	
Bornyl acetate	259	1283.5	11.1	1285	1282–1288	1264–1297	
Neryl formate	3	1285.0	20.1			1268–1307	

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TABLE 4. Retention indices of essential oil components for dimethylsilicone stationary phase with 5% phenyl groups—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
Anethole, (E)-	50	1285.2	8.0	1284	1283–1287	1273–1303	
Isobornyl acetate	73	1285.9	8.5	1286	1284–1288	1271–1302	
Safrole	40	1286.7	3.7	1287	1285–1288	1280–1294	
p-Cymen-7-ol	46	1287.7	8.1	1287	1286–1291	1271–1298	
Lavandulyl acetate	29	1289.2	6.0	1289	1288–1291	1279–1300	
Thymol	225	1290.1	11.2	1291	1290–1293	1272–1304	
2-Undecanone	111	1293.1	6.7	1294	1291–1296	1281–1303	
Menthyl acetate	13	1295.8	7.8	1294		1278–1310	
2,4-Decadienal, (2E,4Z)-	64	1296.3	7.7	1295	1291–1298	1287–1310	
Perilla alcohol	27	1296.3	8.5	1295	1294–1302	1280–1309	
Indole	58	1298.4	12.3	1295	1289–1303	1285–1329	
Carvacrol	223	1300.4	7.3	1299	1298–1302	1291–1314	
Terpinen-4-ol acetate	10	1302.1	15.2	1300		1281–1328	
Geranyl formate	13	1303.1	7.4	1301		1292–1322	
Undecanal	107	1306.5	7.6	1307	1305–1310	1295–1319	
Nonyl acetate	16	1309.2	5.9	1308		1302–1325	
Guaiacol, p-vinyl-	81	1317.4	8.2	1316	1312–1321	1308–1334	1309 (Ref. 7)
2,4-Decadienal, (2E,4E)-	184	1317.6	9.7	1317	1314–1321	1305–1334	
Methyl geranate	23	1323.1	4.6	1323	1322–1325	1316–1331	
Methyl decanoate	32	1325.5	1.7	1326	1324–1327	1323–1329	
Myrtenyl acetate	12	1328.6	5.2	1327		1322–1337	
Bicycloelemene	14	1333.3	7.9	1335.5		1316–1346	
Linalool propanoate	4	1336.0	3.6			1333–1340	1338–1339 (Ref. 40)
Carvyl acetate, trans-	23	1336.6	4.1	1337	1337–1339	1328–1342	
δ-Elemene	150	1337.0	5.8	1338	1335–1340	1327–1344	
Piperitenone	22	1340.7	5.7	1343	1339–1344	1329–1347	
α-Terpinyl acetate	133	1347.0	9.4	1350	1344–1351	1329–1358	
α-Cubebene	256	1351.4	10.8	1351	1348–1352	1340–1373	(d)
α-Longipinene	38	1352.1	8.4	1352.5	1348–1357	1337–1362	(d)
Citronellyl acetate	82	1352.4	6.4	1354	1350–1355	1337–1358	
Thymol acetate	26	1356.4	4.4	1355	1353–1358	1350–1364	
Eugenol	240	1357.8	8.7	1357	1355–1360	1345–1375	
Carvyl acetate, cis-	14	1362.0	3.3	1362		1352–1366	
Neryl acetate	117	1362.9	8.9	1364	1360–1366	1345–1378	
γ-Nonalactone	54	1363.5	11.3	1363	1359–1370	1344–1380	
2-Undecenal, (E)-	46	1364.6	8.2	1365	1361–1370	1351–1379	1357 (Ref. 7)
Piperitenone oxide	13	1366.5	3.1	1366		1363–1373	
Cyclosativene	66	1368.2	5.5	1368	1364–1370	1360–1380	(d)
Nepetalactone, 4aα,7α,7aα	5	1369.2	4.3	1370		1365–1375	1357 (Ref. 7)
α-Ylangene	114	1369.9	7.1	1372	1368–1373	1351–1377	(d)
Carvacrol acetate	14	1373.1	6.5	1371.5		1364–1391	
1-Undecanol	21	1373.6	7.5	1371	1370–1378	1366–1387	1374 (Ref. 40)
Methyl cinnamate, trans-	17	1375.4	9.5	1379		1352–1386	
Decanoic acid	66	1375.5	11.3	1373	1369–1381	1367–1399	1364 (Ref. 7)
α-Copaene	524	1376.2	9.2	1376	1374–1378	1363–1391	
Longicyclene	18	1376.9	8.1	1374.5	1372–1378	1370–1394	
Geranyl acetate	156	1379.9	8.6	1382	1379–1384	1358–1388	
Daucene	8	1380.6	2.1	1380		1378–1384	
4,5-Epoxy-2-decenal, (E)-	59	1380.9	4.6	1381	1379–1384	1374–1390	
α-Isocomene	6	1382.7	9.8	1386.5		1365–1392	(d)
β-Bourbonene	281	1384.2	10.0	1384	1382–1387	1366–1398	
β-Damascenone, (E)-	158	1385.5	7.9	1386	1381–1390	1370–1397	
β-Cubebene	183	1386.6	8.1	1389	1387–1390	1370–1393	
β-Elemene	368	1390.4	9.0	1391	1388–1393	1374–1402	
Jasmone, (Z)-	37	1394.6	8.4	1394	1394–1399	1377–1404	
Ethyl decanoate	50	1395.0	5.7	1396	1394–1398	1383–1403	
Isoitalicene	3	1396.7	1.5	1397		1395–1398	

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TABLE 4. Retention indices of essential oil components for dimethylsilicone stationary phase with 5% phenyl groups—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
Cyperene	28	1397.8	5.4	1399	1397–1400	1386–1406	(d)
Methyl eugenol	119	1401.8	7.4	1402	1400–1406	1394–1410	
Italicene	16	1401.9	3.2	1402	1400–1404	1397–1407	(d)
Vanillin	94	1404.7	11.9	1403	1397–1410	1390–1430	1393 (Ref. 7)
Caryophyllene, (Z)-	53	1406.5	8.9	1405	1404–1409	1392–1426	
Longifolene	66	1406.8	12.6	1404.5	1400–1413	1387–1434	
Decyl acetate	25	1407.1	7.1	1408	1406–1410	1392–1418	
Dodecanal	94	1408.1	6.6	1408	1405–1412	1397–1420	
α-Gurjunene	143	1408.6	9.4	1409	1407–1411	1394–1421	
α-Cedrene	70	1412.2	10.2	1410	1408–1415	1397–1435	(d)
α-Bergamotene, cis-	50	1414.5	8.7	1415	1409–1416	1403–1433	
Caryophyllene, (E)-	741	1420.1	10.4	1419	1417–1422	1405–1440	
2,5-Dimethoxy-p-cymene	10	1421.4	3.2			1415–1425	
β-Ylangene	11	1421.7	1.4	1421		1420–1425	
α-Santalene	20	1421.8	9.0	1420	1417–1422	1413–1441	
β-Cedrene	47	1422.4	6.6	1421	1418–1424	1415–1434	(d)
α-Ionone, (E)-	37	1425.6	8.7	1426	1426–1430	1403–1435	
β-Gurjunene	179	1431.2	13.5	1432	1428–1433	1408–1459	(d)
Thujopsene, cis-	34	1432.0	8.8	1429	1426–1434	1424–1450	(d)
β-Copaene	53	1433.1	7.3	1432	1430–1433	1426–1449	
α-Bergamotene, trans-	141	1434.5	8.4	1436	1432–1438	1416–1444	
γ-Elemene	112	1436.4	19.6	1433	1430–1437	1410–1486	
α-Guaiene	88	1439.6	8.8	1440	1438–1443	1424–1454	(d)
Aromadendrene	222	1440.6	13.0	1439	1437–1443	1419–1465	(d)
β-Humulene	14	1442.5	6.9	1439.4		1436–1456	(d)
α-Himachalene	27	1445.1	7.6	1448	1444–1450	1428–1453	
β-Farnesene, cis-	75	1445.9	6.7	1444	1442–1448	1438–1460	(d)
Geranylacetone	101	1451.8	7.9	1453	1451–1455	1435–1461	
Neryl propanoate	3					1430–1452	1452 (Ref. 7); 1451 (Ref. 52)
α-Humulene	573	1453.1	10.3	1454	1450–1456	1435–1470	
β-Farnesene, (E)-	237	1455.9	7.9	1457	1454–1459	1439–1467	
α-Patchoulene	12	1457.2	4.9	1457		1450–1464	
β-Santalene	23	1458.5	9.9	1461	1452–1464	1443–1474	
Alloaromadendrene	266	1459.9	10.0	1461	1458–1463	1443–1477	
Muurola-4 (14),5-diene, cis-	42	1463.6	8.7	1462	1460–1467	1448–1478	
β-Acoradiene	25	1465.5	9.6	1466	1463–1471	1447–1478	
2-Dodecenal, (E)-	15	1468.4	9.1	1468		1452–1483	
γ-Decalactone	40	1470.6	14.1	1470	1466–1475	1444–1495	
γ-Gurjunene	68	1472.2	8.2	1473	1470–1475	1455–1485	
1-Dodecanol	37	1472.8	7.9	1473	1470–1476	1459–1487	
Undecanoic acid	5	1474.4	11.1			1465–1490	
γ-Himachalene	22	1475.9	7.5	1476	1474–1479	1468–1483	
γ-Muurolene	292	1476.2	8.9	1477	1474–1479	1461–1487	
Geranyl propanoate	9	1476.8	3.6			1473–1485	
β-Chamigrene	39	1478.9	8.1	1476	1475–1481	1471–1496	
γ-Curcumene	46	1480.3	4.5	1480	1478–1483	1474–1488	
Germacrene D	516	1480.6	8.8	1480	1479–1484	1464–1493	
Ar-Curcumene	119	1482.2	7.6	1483	1479–1485	1468–1494	
α-Amorphene	45	1482.4	12.1	1483	1474–1485	1466–1506	
β-Ionone, (E)-	143	1485.9	7.3	1485	1484–1490	1470–1498	
β-Selinene	256	1486.1	8.7	1486	1484–1490	1473–1496	
β-guaiene, cis-	54	1488.8	7.4	1490	1487–1492	1476–1500	
Cubebol, epi-	33	1488.9	11.4	1493	1489–1494	1460–1498	
Phenylethyl 3-methylbutanoate	13	1490.5	4.1	1490		1482–1499	
α-Farnesene, (Z,E)-	22	1490.9	3.9	1491	1488–1493	1486–1497	
Valencene	121	1491.7	8.8	1492	1489–1495	1477–1507	
Viridiflorene	85	1492.2	8.9	1493	1489–1496	1476–1505	

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TABLE 4. Retention indices of essential oil components for dimethylsilicone stationary phase with 5% phenyl groups—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
α-Selinene	136	1493.4	9.7	1494	1490–1497	1477–1510	
Bicyclogermacrene	302	1494.1	8.7	1495	1492–1498	1477–1503	
α-Zingiberene	60	1495.3	6.7	1495	1493–1497	1485–1509	
δ-Decalactone	57	1498.0	12.9	1496	1492–1505	1473–1520	
α-Muurolene	304	1498.3	9.1	1499	1497–1501	1480–1509	
β-Guaiene, trans-	29	1499.2	8.8	1500	1499–1503	1478–1511	
2-Tridecanone	31	1499.4	12.2	1497	1494–1503	1483–1524	
β-Himachalene	30	1501.0	9.1	1499	1497–1503	1491–1523	(d)
Germacrene A	79	1502.1	7.4	1504	1501–1506	1486–1510	
α-Bisabolene, (Z)-	21	1503.1	4.6	1504	1502–1505	1495–1509	
α-Farnesene, (E,E)-	217	1504.1	12.3	1508	1503–1510	1472–1516	
α-Bulnesene	39	1504.1	7.6	1505	1503–1508	1490–1516	
Cuparene	23	1506.6	8.1	1505	1502–1512	1498–1523	
β-Bisabolene	243	1508.4	9.0	1509	1506–1510	1494–1525	
Tridecanal	35	1511.6	6.1	1511	1506–1515	1503–1524	
γ-Bisabolene, (Z)-	25	1511.6	6.4	1515	1507–1515	1502–1518	
β-Curcumene	24	1512.9	3.7	1512.5	1511–1516	1506–1517	
γ-Cadinene	349	1513.1	10.8	1513	1511–1515	1498–1531	
Geranyl isobutanoate	8	1514.4	2.1	1514		1511–1518	
Cubebol	46	1514.9	6.9	1515	1513–1517	1503–1529	
α-Selinene, 7-epi-	35	1517.2	4.9	1517	1515–1519	1509–1525	
Myristicin	28	1518.4	7.7	1519	1515–1523	1503–1528	
Calamenene, cis-	95	1522.9	8.9	1521	1519–1526	1511–1541	1528 (Ref. 7); 1540 (Ref. 53)
δ-Cadinene	551	1523.2	10.1	1524	1520–1525	1508–1539	
β-Sesquiphellandrene	79	1523.5	5.5	1524	1523–1526	1512–1530	
Eugenol acetate	9	1523.7	4.4	1524		1514–1531	
Calamenene, trans-	42	1528.3	7.1	1529	1528–1532	1515–1536	1521 (Ref. 7); 1529 (Ref. 53)
Citronellyl butanoate	10	1528.6	5.6	1530		1513–1532	
Cadina-1(2),4-diene, cis	95	1531.0	6.6	1532	1530–1533	1515–1542	1495 (Ref. 7)
γ-Bisabolene, (E)-	37	1532.9	4.8	1533	1531–1535	1526–1540	
α-Cadinene	130	1533.3	10.9	1537	1534–1538	1503–1541	
α-Calacorene	160	1540.3	8.6	1542	1539–1545	1522–1549	
α-Bisabolene, (E)-	8	1540.3	5.7	1541		1530–1547	
Selina-3,7(11)-diene	28	1540.5	4.8	1542	1539–1544	1531–1546	
Sesquisabinene hydrate, cis-	14	1541.1	10.2	1542.5		1524–1562	
Nerolidol, (Z)-	39	1543.6	14.8	1535	1534–1558	1527–1567	
Elemol	117	1547.5	7.7	1549	1546–1550	1534–1557	
β-Elemol	1						1547 (Ref. 54)
Germacrene B	177	1550.9	18.9	1556	1552–1560	1499–1568	
Elemicin	35	1553.6	6.6	1554	1552–1559	1542–1562	
β-Calacorene	48	1559.4	8.3	1563	1555–1564	1542–1566	
Nerolidol, (E)-	232	1560.9	9.1	1564	1560–1565	1539–1570	
Geranyl butanoate	16	1562.6	3.8	1562.5		1554–1570	
Palustrol	4	1566.8	4.2	1567.5		1561–1571	
Ledol	66	1566.8	14.3	1565		1549–1599	(d); 1602 (Ref. 7); 1569 (Ref. 53)
Caryophyllenyl alcohol	21	1568.6	5.9	1568	1562–1570	1556–1573	
Dodecanoic acid	64	1569.2	9.1	1568	1566–1573	1557–1587	
3-Hexenyl benzoate, (Z)-	42	1569.5	8.8	1570	1567–1572	1552–1588	
Germacrene-D-4-ol	81	1574.2	6.6	1574	1573–1576	1560–1582	
Spathulenol	607	1576.4	9.8	1576	1574–1578	1562–1590	
Dendrolasin	10	1576.5	4.8	1574		1571–1585	
β-Copaen-4α-ol	19	1580.2	10.3	1585		1556–1594	
Caryophyllene oxide	498	1580.6	9.8	1581	1578–1583	1563–1595	
Hexyl benzoate	11	1581.8	7.6	1579		1574–1596	
Globulol	151	1581.8	7.4	1583	1579–1585	1568–1592	
Gleenol	8	1582.8	6.2	1585		1572–1589	
Sesquisabinene hydrate, trans-	7	1583.4	8.5	1581		1571–1598	

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TABLE 4. Retention indices of essential oil components for dimethylsilicone stationary phase with 5% phenyl groups—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
Globulol, epi-	22	1584.8	10.6	1585	1580–1588	1564–1608	
β-Phenylethyl tiglate	8	1590.0	6.1	1588.5		1584–1600	
Viridiflorol	144	1590.8	9.1	1590	1589–1594	1569–1604	
Longiborneol	9	1591.7	4.3	1592		1583–1599	(d)
Ethyl dodecanoate	39	1593.3	5.3	1595	1591–1597	1580–1598	
Salvial-4(14)-en-1-one	24	1593.4	4.2	1595	1589–1595	1587–1599	
Carotol	14	1595.3	3.3	1594		1591–1603	
Guaiol	79	1597.1	8.4	1596	1594–1600	1585–1615	
Geranyl isovalerate	7	1599.3	11.0	1604		1582–1613	
Cedrol	47	1600.1	10.0	1597	1596–1603	1587–1616	(d)
α-Humulene oxide	6	1601.5	2.7	1601.5		1598–1605	
β-Oplopenone	33	1604.0	7.2	1606	1601–1608	1589–1611	
Humulene epoxide II	133	1604.7	6.7	1606	1604–1608	1592–1610	
Tetradecanal	66	1612.3	5.1	1611	1609–1615	1605–1623	
Cubenol, 1,10-di-epi-	60	1612.3	8.7	1614	1611–1616	1591–1623	
γ-Eudesmol, 10-epi-	44	1618.7	4.7	1619	1617–1621	1612–1625	
Dill apiole	26	1621.7	8.6	1622	1620–1625	1608–1634	
1-Cubenol, epi-	110	1625.5	7.1	1627	1625–1629	1611–1631	
α-Acorenol	16	1630.0	3.1	1630		1621–1634	
γ-Eudesmol	95	1630.9	6.2	1631	1629–1632	1623–1643	
Isospathulenol	21	1633.5	7.0	1637	1630–1639	1621–1641	
Cubenol	99	1636.5	11.5	1642	1630–1643	1612–1647	
α-Cadinol, epi-	197	1637.8	7.7	1640	1635–1641	1624–1648	
Caryophylla-4(12),8(13)-dien-5α-ol	6	1640.3	9.3	1640		1627–1656	
α-Muurolol, epi-	164	1640.8	9.6	1642	1640–1644	1623–1654	
α-Muurolol	175	1642.9	10.7	1645	1642–1646	1620–1656	
Himachalol	11	1649.4	10.1	1647		1635–1675	
β-Eudesmol	163	1650.1	8.7	1649	1647–1652	1637–1664	
α-Eudesmol	90	1651.7	9.6	1652	1650–1655	1633–1666	
α-Cadinol	297	1651.9	9.5	1653	1651–1655	1635–1664	
Selin-11-en-4α-ol	39	1654.9	4.1	1653	1652–1660	1649–1660	
Caryophyllenol II	6	1659.7	18.3			1633–1676	
Patchouli alcohol	5	1659.8	4.3	1660		1653–1664	
Bulnesol	31	1665.7	5.3	1666	1666–1668	1655–1672	
Intermedeol	5	1666.2	8.2	1667		1654–1677	
Tridecanoic acid	6	1668.9	8.1			1662–1680	
Cadalene	58	1671.3	8.4	1674	1671–1675	1652–1680	
Valeranone	20	1671.8	2.7	1672	1670–1672	1667–1676	
β-Bisabolol	46	1672.0	5.5	1671	1670–1673	1662–1684	
1-Tetradecanol	24	1676.3	5.1	1676	1673–1680	1668–1686	
α-Bisabolol	112	1682.8	9.0	1684	1681–1686	1665–1698	
α-Bisabolol, epi-	37	1685.3	4.3	1686	1684–1688	1679–1691	
Eudesma-4(15),7-dien-1β-ol	18	1688.0	2.6	1688		1685–1694	
Eudesm-7(11)-en-4-ol	20	1692.3	6.9	1692	1688–1700	1681–1700	
β-Sinensal	14	1694.0	10.9	1695		1669–1707	
Farnesol, (2Z,6Z)-	21	1694.4	7.4	1697	1695–1698	1678–1700	(g); 1698 (Ref. 7); 1718 (Ref. 53)
2-Pentadecanone	26	1699.1	9.1	1698	1696–1703	1685–1716	
Geranyl tiglate	5	1700.8	4.0	1700		1695–1705	
Farnesol, (2E,6Z)-	23	1713.6	6.0	1713	1712–1718	1702–1722	(g); 1714 (Ref. 7); 1746 (Ref. 53)
Pentadecanal	49	1714.4	7.4	1714	1712–1717	1703–1728	
Farnesol, (2Z,6E)-	53	1722.5	5.6	1722	1721–1724	1715–1732	(g); 1722 (Ref. 7); 1701 (Ref. 53)
Methyl tetradecanoate	34	1723.3	7.6	1725	1722–1727	1706–1733	
Chamazulene	18	1726.7	10.1	1725		1708–1749	
Farnesol, (2E,6E)-	19	1743.5	3.4	1743		1736–1750	(g); 1742 (Ref. 7); 1725 (Ref. 53)
α-Sinensal	15	1753.5	6.7	1752		1741–1765	
Benzyl benzoate	79	1761.3	13.3	1762	1759–1766	1735–1785	
Tetradecanoic acid	79	1767.3	9.4	1796	1763–1771	1749–1782	

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TABLE 4. Retention indices of essential oil components for dimethylsilicone stationary phase with 5% phenyl groups—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
Ethyl tetradecanoate	26	1793.9	3.4	1793.5	1793–1795	1790–1798	
Nootkatone	27	1813.4	17.9	1814	1799–1828	1783–1837	
Hexadecanal	41	1816.5	8.1	1817	1811–1820	1807–1830	
Farnesyl acetate, (2E,6E)-	18	1842.3	3.5	1843		1836–1850	
Hexahydrofarnesylacetone	93	1844.4	7.5	1845	1843–1847	1831–1855	
Benzyl salicylate	14	1867.4	8.4	1863		1857–1881	
Pentadecanoic acid	33	1867.8	9.1	1868	1863–1872	1854–1883	
1-Hexadecanol	49	1879.7	5.7	1880	1876–1882	1870–1892	
2-Heptadecanone	13	1903.4	6.8	1902		1892–1915	
Farnesyl acetone, (5E,9E)	4	1919.5	1.3			1918–1921	
Methyl hexadecanoate	83	1924.2	6.4	1926	1922–1927	1910–1931	
Isophytol	40	1946.8	4.2	1948	1943–1949	1939–1951	
Hexadec-9-enoic acid, (Z)-	6	1951.1	8.0	1953		1936–1958	
Hexadecanoic acid	145	1968.4	14.3	1968	1962–1973	1939–1996	1959 (Ref. 7)
Ethyl hexadecanoate	41	1991.5	9.3	1993	1990–1996	1975–2000	
Manoyl oxide	48	1993.1	9.2	1991	1989–1998	1978–2010	(d)
Manool, 13-epi-	24	2010.2	5.7	2010.5	2010–2013	1999–2017	
Abietatriene	29	2054.3	3.4	2054	2054–2057	2051–2058	
Manool	32	2057.3	6.5	2056	2055–2057	2049–2069	
Abietadiene	21	2080.5	8.7	2080	2080–2082	2064–2088	2087 (Ref. 7)
1-Octadecanol	26	2082.8	3.5	2082	2080–2084	2078–2090	
Methyl linoleate	31	2091.1	6.4	2092	2089–2095	2079–2099	
Methyl oleate	14	2096.1	8.4	2097		2082–2109	
Phytol	40	2116.4	10.2	2114	2110–2122	2104–2136	1942 (Ref. 7)
Methyl octadecanoate	46	2126.7	9.1	2128	2125–2133	2110–2139	
Linoleic acid	29	2128.9	20.3	2130	2114–2144	2097–2158	
Oleic acid	22	2133.2	20.5	2137	2115–2147	2102–2161	
Ethyl linoleate	14	2158.8	7.8	2159		2144–2177	
Octadecanoic acid	33	2172.4	8.7	2172	2167–2178	2159–2184	

Comments: (a) Number of data records. (b) See (b) in Table 3. (c) See (c) in Table 3. (d) Observed RI values were close for dimethylsilicone and 5%phenylmethylsilicone stationary phases, or the retention index was higher for dimethylsilicone phase. (e) See (e) in Table 3. (f) See (f) in Table 3. (g) See (i) in Table 3.

TABLE 5. Retention indices of essential oil components for polar phase

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
Ethyl acetate	192	886.4	14.3	889	879–896	858–908	
Butanal, 2-methyl-	97	915.5	14.1	915	907–922	894–943	
3-Methylbutanal	152	921.5	11.9	920	913–929	906–943	
2-Ethylfuran	42	953.2	9.2	951.5	945–960	941–965	
Pentanal	108	975.3	20.3	979	967–986	935–1003	
2,3-Butanedione	199	977.6	15.1	980	968–986	954–1000	
Tricyclene	65	1012.4	8.1	1014	1007–1015	998–1029	
α-Pinene	488	1025.4	10.4	1026	1018–1032	1008–1039	
α-Thujene	206	1026.6	9.3	1027	1020–1035	1012–1039	
Ethyl butanoate	208	1035.7	12.4	1035	1027–1043	1019–1057	
Santolina triene	7	1036.1	16.9	1042		1011–1063	
α-Fenchene	59	1061.0	12.5	1060	1053–1070	1044–1084	
Ethyl isovalerate	89	1066.9	11.5	1068	1060–1074	1047–1084	
Camphene	311	1068.5	13.2	1069	1060–1076	1043–1086	
Hexanal	464	1082.0	15.5	1083	1075–1091	1056–1106	
Isobutanol	222	1089.3	16.7	1091	1081–1099	1057–1113	
β-Pinene	436	1110.0	13.3	1111.5	1102–1118	1085–1130	
Isopentyl acetate	140	1121.4	10.6	1121	1114–1129	1102–1140	

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TABLE 5. Retention indices of essential oil components for polar phase—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
Thuja-2,4(10)-diene	5	1122.0	11.6	1117		1109–1137	(d)
Sabinene	340	1122.0	13.3	1124	1115–1132	1098–1140	
Verbenene	9	1123.8	5.2	1123		1118–1131	
δ-2-Carene	13	1133.9	12.4	1137		1110–1150	
Ethyl pentanoate	57	1136.1	11.8	1134	1127–1141	1121–1161	
3-Hexenal, (Z)-	68	1139.1	12.2	1138.5	1132–1147	1118–1160	
1-Butanol	231	1139.6	16.9	1140	1127–1150	1113–1167	
3-Carene	171	1146.8	17.4	1147	1140–1152	1122–1169	
1-Penten-3-ol	120	1157.7	15.6	1158	1147–1166	1130–1179	
Myrcene	491	1160.9	11.2	1161	1155–1169	1140–1175	
α-Phellandrene	240	1167.7	12.5	1167	1160–1176	1148–1186	
α-Terpinene	300	1177.8	14.9	1180	1170–1188	1154–1195	
2-Heptanone	150	1182.3	13.2	1183	1173–1191	1160–1205	
Methyl hexanoate	63	1184.6	9.3	1184	1177–1191	1172–1202	
Heptanal	208	1185.1	13.2	1186	1177–1194	1163–1208	
1,4-Cineole	22	1186.3	12.9	1185	1177–1197	1169–1212	
2-Methylpropyl 3-methylbutanoate	12	1186.4	12.7	1187		1165–1199	
Dehydro-1,8-cineole	14	1192.5	7.8	1195		1167–1197	
Limonene	640	1198.2	13.4	1200	1190–1204	1178–1219	
Butan-1-ol, 2-methyl-	102	1205.8	11.8	1208	1200–1212	1182–1223	
3-Methyl-1-butanol	302	1206.9	16.6	1209	1198–1217	1179–1236	
β-Phellandrene	249	1209.3	15.1	1210	1202–1218	1188–1233	
1,8-Cineole	307	1211.1	14.6	1212	1203–1220	1186–1231	
2-Hexenal, (E)-	231	1216.3	12.2	1215	1208–1224	1196–1238	
2-Pentylfuran	131	1232.1	11.6	1232	1224–1241	1213–1249	
Ethyl hexanoate	223	1233.4	12.8	1232	1224–1241	1216–1258	
β-Ocimene, (Z)-	248	1234.5	12.4	1235	1228–1246	1211–1251	
γ-Terpinene	381	1245.0	13.6	1246	1238–1255	1222–1266	
1-Pentanol	235	1247.1	15.7	1250	1238–1256	1217–1271	
β-Ocimene, (E)-	310	1250.4	12.7	1250	1244–1257	1232–1267	
3-Octanone	84	1254.8	15.7	1254.5	1244–1265	1230–1280	
Styrene	87	1261.5	14.9	1262	1251–1270	1240–1290	
p-Cymene	461	1270.1	12.9	1272	1264–1280	1246–1291	(e); 1279 (Ref. 41); 1280 (Ref. 55); 1266 (Ref. 6)
Hexyl acetate	151	1273.5	13.2	1272	1265–1280	1254–1298	
m-Cymene	19	1277.0				1244–1279	(e); average of data (Refs. 41 and 55); 1264 (Ref. 6)
Acetoin	198	1282.2	19.9	1282	1270–1294	1250–1314	
Terpinolene	369	1282.4	11.6	1283	1277–1290	1261–1300	
Octanal	319	1287.2	13.3	1289	1278–1296	1267–1312	
Isopentyl isovalerate	28	1293.8	11.4	1292.5	1285–1304	1278–1312	
1-Octen-3-one	178	1301.0	12.5	1300	1293–1309	1280–1324	
o-Cymene	18					1248–1310	(e); 1310 (Ref. 41); 1298 (Ref. 56)
2-Heptanol	75	1315.3	16.8	1320	1304–1326	1284–1335	
2-Pentenol, (Z)-	63	1315.7	12.1	1317	1310–1324	1296–1334	1323 (Ref. 6)
3-Hexenyl acetate, (Z)-	111	1315.9	9.4	1315	1310–1321	1301–1335	
2-Buten-1-ol, 3-methyl-	38	1316.1	17.5	1320	1310–1328	1280–1338	
2-Heptenal, (E)-	72	1321.6	15.1	1321	1314–1335	1289–1339	
2-Hexen-1-ol, acetate, (E)-	37	1332.2	10.3	1333	1323–1338	1315–1348	
6-Methyl-5-hepten-2-one	179	1336.9	12.5	1338	1329–1346	1317–1357	
Artemisia ketone	12	1344.7	11.9	1348		1320–1358	
Rose oxide, cis-	31	1350.1	12.1	1350	1338–1358	1331–1369	
1-Hexanol	294	1351.4	17.0	1354	1344–1360	1316–1377	
α-Pinene oxide	8	1363.9	19.9			1331–1384	(d); 1384 (Ref. 57); 1354–1371 (Ref. 40)
allo-Ocimene	19	1366.5	16.5	1367		1334–1394	(f); 1394 (Ref. 58)
Rose oxide, trans-	13	1367.3	12.1	1367		1341–1386	
3-Hexen-1-ol, (E)-	171	1372.8	17.0	1371	1364–1385	1344–1399	

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TABLE 5. Retention indices of essential oil components for polar phase—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
Dimethyl trisulfide	139	1376.2	16.7	1377	1365–1386	1347–1406	
1-Octen-3-yl acetate	8	1379.7	11.2			1365–1402	
3-Hexen-1-ol, (Z)-	251	1380.2	15.3	1382	1370–1390	1351–1405	
α-Isocomene	10	1388.1	7.9	1388		1377–1405	
Methyl octanoate	50	1388.8	11.2	1386.5	1379–1398	1375–1410	
2-Nonanone	106	1391.3	11.7	1391	1384–1397	1374–1415	
Nonanal	377	1391.5	12.5	1391	1385–1400	1370–1414	
3-Octanol	94	1391.9	11.8	1393	1386–1398	1372–1408	
Yomogi alcohol	11	1395.1	10.8	1403		1377–1405	
Fenchone	31	1399.5	10.9	1397	1391–1410	1386–1418	
2-Hexen-1-ol, (E)-	125	1399.9	14.5	1404	1389–1410	1377–1419	
2,4-Hexadienal-, (2E,4E)-	27	1401.7	18.7	1400	1395–1409	1371–1438	
1,3,8-p-Menthatriene	16	1411.0	24.5	1408		1375–1453	(d)
Hexyl butanoate	50	1414.1	12.9	1414	1406–1425	1395–1433	
Thujone, cis-	47	1423.1	16.6	1429	1417–1434	1385–1441	
Perillene	18	1425.3	8.3	1429		1405–1431	(g); 1429 (Ref. 59)
Hexyl 2-methyl butanoate	16	1428.1	8.4	1432		1415–1438	1438 (Ref. 60)
2-Octenal, (E)-	122	1429.5	14.6	1429.5	1421–1437	1407–1463	
p-Methyl anisole	9	1431.7	12.7	1432		1409–1446	
Ethyl octanoate	172	1434.9	12.3	1434.5	1428–1441	1416–1458	
p-Cymenene	69	1437.5	15.3	1437	1429–1452	1412–1457	
Thujone, trans-	41	1439.6	16.1	1442	1436–1451	1400–1452	
1-Octen-3-ol	273	1444.2	17.3	1450	1437–1454	1411–1465	
Linalool oxide, (furanoid), cis-	155	1446.0	22.3	1445	1427–1465	1410–1478	
Acetic acid	314	1446.1	20.5	1449	1433–1460	1408–1479	1427–1443 (Ref. 40)
1-Heptanol	110	1448.8	14.6	1452	1440–1460	1419–1467	
Limonene oxide, cis-	39	1450.5	11.0	1453	1443–1458	1429–1466	
Linalool oxide, (furanoid), trans-	157	1454.3	15.1	1451	1446–1464	1429–1481	
Methional	187	1456.1	16.2	1453	1448–1465	1430–1484	
3-Hexenyl butanoate, (Z)-	30	1456.1	10.6	1455	1448–1463	1444–1473	
Sabinene hydrate, cis-	111	1460.2	15.1	1463	1456–1469	1425–1478	(h)
α-Cubebene	161	1460.4	12.8	1463	1455–1468	1438–1480	
Furfural	213	1460.9	16.1	1461	1450–1471	1432–1490	
Limonene oxide, trans-	38	1461.6	12.1	1465.5	1454–1468	1439–1481	
5-Hepten-2-ol, 6-methyl-	24	1463.8	10.8	1466	1461–1468	1446–1478	
Menthone	40	1465.3	14.4	1473.5	1450–1475	1443–1479	
Nerol oxide	27	1468.6	12.3	1467	1461–1477	1450–1487	
δ-Elemene	77	1468.8	10.6	1470	1464–1479	1447–1481	
α-Longipinene	12					1462–1541	(d,i); 1469 (Ref. 61)
Octanol acetate	57	1474.6	10.9	1475	1467–1483	1459–1491	
Citronellal	87	1475.3	14.5	1477	1465–1487	1457–1495	
Fenchyl acetate, endo-	2					1456–1480	
Menthofuran	9	1482.4	15.1	1487		1458–1502	
Cyclosativene	17	1483.2	9.1	1485		1445–1549	(d,j); 1492 (Ref. 61)
Isomenthone	20	1483.8	16.6	1481.5	1469–1503	1464–1506	
α-Ylangene	59	1484.1	14.7	1490	1474–1493	1459–1500	
Bicycloelemene	38	1487.5	7.7	1485.5	1484–1495	1471–1495	
1-Hexanol, 2-ethyl-	117	1487.9	16.5	1491	1484–1495	1452–1513	
Longicyclene	5	1489.4	8.6	1494		1480–1497	
Isoitalicene	6	1490.5	8.2	1491		1475–1498	
2,4-Heptadienal, (2E,4E)-	107	1491.0	18.1	1494	1483–1505	1455–1514	
α-Copaene	326	1491.0	17.1	1492	1481–1497	1462–1522	
Daucene	5	1495.2	8.8	1495		1486–1504	
Decanal	227	1495.9	15.3	1497	1485–1506	1471–1516	
α-Campholenal	64	1496.0	10.3	1499	1488–1500	1477–1511	
2-Acetylfuran	110	1498.8	16.6	1499	1489–1510	1468–1531	
Tagetone, (E)-	3					1436–1522	1501 (Ref. 45)

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TABLE 5. Retention indices of essential oil components for polar phase—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
2-Nonenal, (Z)-	54	1501.9	13.1	1500	1492–1512	1480–1529	
Chrysanthenone	11	1507.6	14.1	1510		1482–1522	(d); 1522 (Ref. 62)
Artemisia alcohol	13		12.8	1510		1476–1523	(d,k)
Camphor	177	1515.1	18.1	1518	1507–1532	1481–1537	
Tagetone, (Z)-	4					1459–1580	1517 (Ref. 45)
Benzaldehyde	390	1518.7	22.7	1520	1504–1533	1481–1555	
2-Nonanol	41	1519.6	16.7	1521	1511–1532	1484–1538	1528 (Ref. 6)
Pinene hydrate, trans-	1						1522 (Ref. 63)
β-Bourbonene	135	1523.2	15.3	1526	1515–1535	1496–1546	
Pinocamphone, trans	14	1523.4	14.3	1524		1504–1548	
Cyperene	10	1528.0	7.8	1528		1514–1540	
α-Gurjunene	82	1529.1	11.4	1527.5	1523–1538	1511–1545	
β-Guaiene, trans-	2					1532–1643	
2-Nonenal, (E)-	178	1535.9	16.5	1535	1526–1547	1509–1569	
β-Cubebene	116	1541.7	12.3	1545	1536–1549	1518–1560	
Italicene	6					1489–1543	(d)
Linalool	675	1543.3	16.9	1547	1537–1553	1507–1564	
Pinocamphone, cis	21	1544.6	19.9	1551	1535–1562	1511–1562	
Sabinene hydrate, trans-	55	1548.9	12.1	1551	1542–1556	1526–1565	(h)
1-Octanol	291	1551.6	17.0	1556	1544–1562	1519–1574	
Linalool acetate	91	1554.0	12.5	1555	1548–1565	1532–1570	
Menthyl acetate	10	1554.8	16.7			1535–1585	
α-Bergamotene, cis-	15	1559.1	17.8	1557	1545–1577	1534–1580	
Chrysanthenyl acetate, cis-	10	1561.1	21.5	1559		1533–1590	1582 (Ref. 64)
Sabinene hydrate acetate, cis-	1						1564 (Ref. 65)
Fenchol, endo-	16	1570.0	11.3	1573		1543–1593	
Terpine-1-ol	8	1572.9	9.7			1562–1589	
Isobornyl acetate	20	1572.9	12.6	1577	1564–1584	1551–1585	1564–1585 (Ref. 40)
Nopinone	11	1573.1	19.9	1566		1545–1601	1601 (Ref. 59)
Furfural, 5-methyl-	118	1573.6	22.9	1570	1560–1584	1539–1619	
Pinocarvone	64	1575.5	15.0	1586	1565–1586	1545–1590	
α-Bergamotene, trans-	55	1575.7	10.2	1580	1568–1583	1560–1590	
β-Ylangene	18	1576.9	12.9	1576		1547–1589	
Longifolene	31	1577.3	10.1	1576	1572–1583	1563–1595	
neo-Menthol	14	1578.1	18.7			1551–1604	
Nonyl acetate	19	1578.6	9.9	1581		1560–1603	
Bornyl acetate	168	1579.3	15.6	1580	1570–1592	1549–1597	
β-Copaene	26	1579.8	16.1	1585	1567–1590	1550–1603	(d)
2,6-Nonadienal, (2E,6Z)-	143	1582.2	14.0	1583	1573–1593	1555–1601	
α-Santalene	7	1582.7	11.6	1576		1574–1601	
α-Cedrene	43	1582.9	15.7	1578	1571–1600	1563–1608	
p-Menth-2-en-1-ol, trans-	63	1584.2	22.5	1573	1571–1605	1557–1625	
Myrcenol	17		16.5	1585		1581–1625	(d,k)
Thymol, methyl ether	47	1587.2	15.1	1589	1578–1598	1563–1607	
Caryophyllene, (Z)-	17	1588.2				1570–1685	(l); 1589 (Ref. 66)
β-Elemene	220	1590.9	12.3	1591	1585–1600	1565–1608	
Isophorone	22	1591.2	24.3	1593	1572–1607	1559–1632	(d); 1553–1585 (Ref. 40); 1599 (Ref. 6)
Bornyl formate	9	1595.1	9.8	1588		1588–1610	
Isopulegone, trans-	4	1596.2	2.7			1592–1598	
Methyl decanoate	42	1596.3	14.8	1593.5	1585–1604	1581–1624	
β-Gurjunene	37	1596.7	17.5	1601	1590–1610	1564–1618	
2-Undecanone	83	1598.1	11.7	1598	1593–1604	1579–1617	
Caryophyllene, (E)-	507	1598.5	20.1	1596	1585–1612	1569–1632	
Carvacrol, methyl ether	33	1598.9	15.1	1601	1585–1614	1576–1614	
Terpinen-4-ol	394	1601.2	18.8	1602	1592–1611	1564–1630	
Camphene hydrate	5					1518–1602	1589 (Ref. 67)

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TABLE 5. Retention indices of essential oil components for polar phase—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
Lavandulyl acetate	21	1602.3	10.5	1606	1596–1609	1584–1617	
Hotrienol	30	1602.5	13.8	1607	1588–1615	1580–1616	
Linalool propanoate	9					1596–1696	(d); 1604–1610 (Ref. 40)
Undecanal	57	1605.1	14.1	1604	1595–1614	1582–1630	
2,4-Octadienal-, (2E,4E)-	15	1605.3	16.3	1601		1585–1634	
Sabinene hydrate acetate, trans-	2					1501–1610	1501 (Ref. 68)
2-Octen-1-ol, (E)-	26	1610.3	11.8	1613	1606–1620	1590–1622	
β-Cyclocitral	49	1610.3	17.3	1606	1599–1624	1548–1638	
β-Cedrene	23	1611.1	23.7	1606	1595–1632	1574–1647	
p-Menth-2-en-1-ol, cis-	71	1614.1	35.8	1638	1567–1638	1555–1645	(d); 1638 (Ref. 57)
Citronellyl formate	19	1615.2	15.2	1615		1588–1644	
Methyl benzoate	68	1615.5	21.9	1611.5	1600–1632	1583–1656	
Aromadendrene	115	1620.2	25.2	1620	1604–1629	1583–1668	
Dihydrocarvone, trans-	18	1623.1	17.7	1624		1600–1650	(d,m); 1645 (Ref. 69)
Butanoic acid	235	1623.7	19.2	1624	1613–1636	1593–1655	
α-Bulnesene	38		48.4	1629		1608–1730	(d); 1730 (Ref. 70)
Menthol	50	1630.4	15.8	1636	1618–1641	1599–1651	
Myrtenal	81	1631.5	18.6	1635	1621–1648	1597–1648	
Thujopsene, cis-	10	1631.8	16.2	1627		1606–1660	(d)
Ethyl decanoate	105	1636.2	12.5	1635	1626–1644	1616–1660	
p-Mentha-2,8-dien-1-ol, trans-	29		22.6	1639		1611–1688	(d,k)
β-Terpineol, cis-	5		14.0	1639		1616–1644	(d,k)
γ-Elemene	55	1639.1	13.7	1642	1633–1650	1612–1654	
2-Decenal, (E)-	80	1639.7	19.8	1642	1630–1655	1595–1662	
Terpinen-4-ol acetate	11	1640.1	23.4			1609–1687	(d); 1630 (Ref. 71)
Benzeneacetaldehyde	218	1640.7	22.2	1641	1625–1652	1605–1680	
Umbellulone	12	1641.7	22.3	1646		1610–1667	(d); 1657 (Ref. 55)
Muurola-4 (14),5-diene, cis-	2					1517–1643	
β-Santalene	11	1644.9	15.5			1617–1663	
Acetophenone	107	1647.6	25.4	1645	1631–1660	1607–1699	1660 (Ref. 6)
Alloaromadendrene	136	1649.2	15.5	1649	1638–1661	1624–1668	
Sabina ketone	10					1606–1683	(d); 1651 (Ref. 61)
β-Farnesene, cis-	44	1651.4	15.7	1653	1638–1667	1627–1668	
α-Guaiene	20					1583–1668	(n); 1655 (Ref. 72)
p-Mentha-2,8-dien-1-ol, cis-	16	1652.1	19.1	1649		1620–1678	
Pulegone	35	1654.5	12.5	1661	1651–1662	1626–1663	
1-Nonanol	82	1655.7	14.6	1660	1649–1665	1624–1674	
Furfuryl alcohol	117	1656.3	18.9	1659	1648–1665	1618–1688	
Citronellyl acetate	87	1656.5	13.3	1658	1650–1666	1633–1671	
Isoborneol	27	1659.1	11.8	1660	1654–1665	1635–1675	
Verbenol, cis-	20	1659.8	6.8	1663	1654–1663	1647–1668	
Pinocarveol, trans-	84	1661.2	10.1	1664	1652–1670	1643–1671	
α-Himachalene	14	1663.9	28.6	1652		1632–1723	(d)
β-Farnesene, (E)-	169	1663.9	12.2	1665	1659–1670	1643–1684	
β-guaiene, cis-	14	1663.9	23.9	1667		1621–1702	(d)
Butanoic acid, 2-methyl-	107	1664.5	16.4	1661	1657–1673	1639–1693	
Ethyl benzoate	85	1665.1	21.6	1659.5	1650–1677	1640–1706	
Isovaleric acid	207	1666.5	17.6	1665	1657–1679	1636–1697	1652–1665 (Ref. 40)
α-Humulene	395	1666.7	18.1	1667	1655–1682	1637–1689	
γ-Gurjunene	14	1668.2	11.4	1673		1647–1689	
Salicylaldehyde	26	1670.9	23.5	1674	1658–1685	1629–1704	1644–1667 (Ref. 40)
Methyl chavicol	32	1671.4	12.8	1671	1661–1680	1652–1690	
β-Humulene	5	1673.2	10.7	1674		1660–1689	
p-Mentha-1,5-dien-8-ol	30					1670–1740	(o); 1674 (Ref. 73); 1738 (Ref. 59)
Neryl formate	8	1674.1	22.3			1641–1708	(d)
Cryptone	29	1674.8	15.3	1679	1668–1687	1644–1690	1690 (Ref. 59)
Decyl acetate	30	1677.3	11.9	1677.5	1669–1688	1662–1692	

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TABLE 5. Retention indices of essential oil components for polar phase—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
Neral	147	1678.5	20.5	1679	1668–1693	1641–1706	
δ-Terpineol	37	1679.3	9.2	1682	1680–1684	1655–1687	
Lavandulol	25	1679.4	12.8	1677	1672–1686	1662–1706	
Verbenol, trans-	53	1680.3	7.5	1683	1675–1684	1665–1691	
4-Ketoisophorone	20	1682.5	21.8	1676	1668–1695	1655–1718	(d)
Carvotanacetone	7	1687.7	21.2	1697		1652–1716	
β-Acoradiene	9	1687.7	12.5	1693		1674–1708	
Limonen-4-ol	19	1688.1	16.6	1700		1662–1717	1700 (Ref. 61)
Methyl geranate	7	1688.4	10.4	1686		1678–1701	
γ-Muurolene	143	1689.8	17.2	1691	1679–1704	1655–1714	
Myrtenyl acetate	15	1691.9	10.9	1698		1677–1704	
γ-Curcumene	21	1692.1	8.5	1690	1685–1704	1682–1704	
α-Amorphene	19	1693.1	23.9	1688		1662–1744	
α-Terpineol	507	1694.0	19.2	1697	1682–1706	1659–1724	
α-Terpinyl acetate	90	1694.8	14.9	1692.5	1685–1709	1672–1718	
2,4-Nonadienal, (2E,4E)-	73	1696.1	13.1	1698	1687–1705	1673–1715	
Viridiflorene	68	1696.2	15.6	1697	1694–1704	1658–1712	
Geranyl formate	16	1696.9	17.4	1693		1665–1727	
Borneol	199	1699.6	22.5	1701	1690–1719	1653–1728	
Dihydrocarveol	5	1707.3	9.2			1698–1727	
Germacrene D	286	1708.2	17.1	1710	1699–1726	1676–1726	
γ-Himachalene	7	1708.7	10.2	1705		1696–1723	
Piperitol, trans-	36	1710.4	28.9	1695	1689–1739	1675–1761	1689 (Ref. 74)
Dodecanal	67	1711.5	13.7	1712	1702–1722	1685–1732	
β-Selinene	144	1716.9	18.8	1715	1706–1731	1686–1743	
Sabinol, trans-	8	1717.0	5.0	1719.5		1708–1720	
Neryl acetate	102	1718.1	13.9	1723	1706–1726	1693–1740	
Veratrole	14	1720.3	16.4	1721		1695–1753	
Verbenone	68	1720.5	11.6	1725	1713–1726	1696–1735	
α-Zingiberene	41	1720.7	14.6	1725	1713–1728	1696–1743	
Benzyl acetate	64	1723.1	26.9	1723	1697–1742	1689–1771	
β-Himachalene	16	1723.1		1718		1704–1752	1740 (Ref. 61)
α-Muurolene	173	1723.4	20.4	1726	1714–1740	1686–1753	
Phellandral	14	1723.9	26.4			1687–1770	(d); 1744 (Ref. 74)
β-Chamigrene	10	1723.9	21.5			1686–1755	(d)
Geranial	137	1725.0	19.1	1728	1716–1739	1680–1750	
α-Selinene	113	1725.3	16.1	1725	1716–1740	1696–1748	
Carvyl acetate, trans-	8					1687–1765	(d,p)
β-Bisabolene	138	1727.5	15.4	1727	1718–1741	1698–1748	
α-Farnesene, (Z,E)-	20	1727.9	9.6	1725	1721–1733	1713–1748	
1,4-Dimethoxybenzene	7					1693–1759	(d)
Valencene	60	1728.6	21.9	1727	1717–1740	1688–1761	
Piperitone	66	1729.9	20.5	1736.5	1717–1744	1689–1748	
Carvone	123	1733.6	19.1	1738	1720–1751	1699–1751	
Bicyclogermacrene	186	1734.5	20.0	1734	1723–1751	1692–1757	
Naphthalene	82	1735.6	24.9	1744	1715–1755	1690–1765	
β-Curcumene	14	1737.0	14.1	1738		1711–1756	(d)
Linalool oxide (pyranoid), trans-	43	1738.5	17.1	1739	1725–1750	1716–1770	
α-Bisabolene, (Z)-	11	1740.4	21.1	1740		1702–1772	(d)
α-Farnesene, (E,E)-	153	1743.9	15.1	1745	1735–1755	1714–1763	
γ-Bisabolene, (E)-	6	1744.7	13.9			1727–1761	
Germacrene A	11	1747.4	14.5	1743		1725–1776	
2-Undecenal, (E)-	43	1747.6	21.8	1750	1737–1762	1710–1784	
Piperitol, cis-	58	1750.5	12.1			1668–1771	(q); 1758 (Ref. 59)
γ-Bisabolene, (Z)-	8	1750.5	14.9	1753.5		1726–1773	
Geranyl acetate	178	1751.1	14.7	1752	1743–1764	1728–1772	
1-Decanol	53	1754.7	17.3	1759	1744–1766	1725–1782	

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TABLE 5. Retention indices of essential oil components for polar phase—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
δ-Cadinene	331	1755.7	17.1	1758	1746–1772	1722–1774	
2,4-Decadienal, (2E,4Z)-	53	1756.1	15.5	1755	1746–1768	1729–1779	
Chrysanthenol, cis-	7	1762.0	5.4	1764		1751–1765	
γ-Cadinene	165	1763.3	15.6	1765	1752–1776	1735–1782	
Citronellol	157	1763.9	16.5	1765	1756–1774	1734–1789	
α-Selinene, 7-epi-	5	1764.2	9.1	1762		1754–1775	
Citronellyl butanoate	4					1765–1811	
Methyl salicylate	130	1767.8	28.2	1765	1745–1794	1727–1809	
α-Cadinene	39	1769.1	22.7	1779	1743–1785	1734–1803	
β-Sesquiphellandrene	62	1771.4	11.7	1772.5	1766–1783	1748–1783	
Ar-Curcumene	102	1773.5	14.6	1777	1766–1786	1743–1788	
p-Methylacetophenone	27	1773.8	21.6	1771	1752–1795	1739–1797	1797 (Ref. 70); 1794 (Ref. 45); 1735–1767 (Ref. 40)
Carvyl acetate, cis-	7					1725–1795	(d,r); 1782 (Ref. 75); 1731 (Ref. 72)
α-Bisabolene, (E)-	11	1775.2	8.2	1772		1763–1786	
Neryl propanoate	10	1777.7	9.8	1782		1758–1786	1809–1818 (Ref. 40)
Selina-3,7(11)-diene	12	1783.2	16.1	1790		1750–1800	
Cumin aldehyde	74	1784.1	19.5	1786	1769–1802	1747–1805	
Cadina-1(2),4-diene, cis	54	1788.0	15.6	1786	1773–1799	1764–1810	
Geranyl isobutanoate	12	1789.6	20.3	1784		1761–1821	(d); 1819 (Ref. 74)
Myrtenol	128	1790.4	19.3	1796	1785–1804	1743–1808	
Perilla aldehyde	33	1793.9	16.4	1793	1781–1807	1770–1818	
Nerol	205	1794.6	24.1	1797	1782–1808	1752–1832	
iso-Dihydrocarveol	3					1745–1800	
Sabinol, cis-	9	1800.6	13.3	1800		1782–1820	(s); 1800 (Ref. 55)
1(7),8-p-Menthadien-2-ol, trans-	14	1803.1	13.5	1811		1774–1821	
2-Tridecanone	52	1808.1	11.9	1809	1800–1815	1788–1825	
2,4-Decadienal, (2E,4E)-	176	1808.2	21.5	1810	1792–1827	1770–1834	
2-Phenylethyl acetate	116	1812.9	20.6	1812	1797–1827	1784–1851	
Geranyl propanoate	14	1815.5	11.6	1816		1799–1830	
Cuparene	19	1816.1	23.8	1821		1766–1849	(d)
Tridecanal	25	1818.5	15.0	1824	1809–1830	1792–1833	
β-Damascenone, (E)-	171	1820.9	18.0	1823	1806–1838	1789–1842	
Calamenene, trans-	22	1823.0	13.9	1826	1813–1830	1802–1844	
Germacrene B	63	1823.8	26.8	1820	1805–1854	1778–1854	
Anethole, (E)-	37	1826.1	15.3	1829	1812–1838	1802–1846	
Calamenene, cis-	109	1834.5	15.7	1837	1828–1847	1800–1853	
Carveol, trans-	94	1836.3	13.2	1845	1829–1845	1805–1850	
Geraniol	311	1839.3	22.3	1845	1830–1857	1795–1865	
Ethyl dodecanoate	67	1839.7	14.7	1840	1826–1850	1820–1866	
Hexanoic acid	274	1843.3	20.0	1845	1833–1856	1807–1873	
α-Ionone, (E)-	32	1843.4	30.2	1839.5	1823–1864	1798–1892	
p-Cymen-8-ol	158	1848.3	19.3	1852	1834–1864	1813–1865	
1-Undecanol	21	1853.3	18.9	1853	1840–1871	1822–1876	1855–1866 (Ref. 40)
Carveol, cis-	57	1854.4	22.6	1856	1838–1881	1818–1882	
Methyl 3-phenylpropionate	6	1854.5	7.7	1854.5		1842–1866	
Geranylacetone	91	1854.9	16.2	1859	1847–1868	1820–1873	
o-Guaiacol	165	1859.8	20.7	1860	1848–1873	1826–1894	
Benzyl alcohol	276	1865.3	24.6	1869.5	1852–1881	1821–1905	
2-Dodecenal, (E)-	17	1865.8	18.7	1867		1835–1901	
Thymol acetate	12					1783–1945	(d); 1867 (Ref. 69)
Safrole	18	1868.1	7.6	1871.5		1853–1876	
2,5-Dimethoxy-p-cymene	7	1868.1	19.1			1826–1878	
Cinnamaldehyde, cis-	3					1870–1888	
Geranyl butanoate	13	1879.0	23.9	1877		1833–1907	1883–1893 (Ref. 40)
Carvacrol acetate	3	1880.1	11.1			1868–1890	

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TABLE 5. Retention indices of essential oil components for polar phase—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
1(7),8-p-Menthadien-2-ol, cis-	19	1894.9	11.2	1896		1863–1903	(d)
Cubebol, epi-	34					1854–1928	(t); 1900 (Ref. 59)
2-Phenylethyl alcohol	359	1903.7	25.0	1905	1890–1920	1859–1944	
Geranyl isovalerate	14	1904.1	15.7	1904		1877–1925	
Piperitenone	12	1909.1	38.7			1840–1949	
Phenylacetonitrile	24	1912.1	27.2	1908.5	1893–1933	1871–1957	1885–1918 (Ref. 40)
α-Calacorene	100	1921.4	16.8	1918	1912–1941	1893–1941	
Tetradecanal	40	1926.9	13.7	1933	1920–1934	1901–1944	
Palustrol	30	1930.4	9.3	1934	1931–1938	1911–1938	
β-Ionone, (E)-	165	1935.5	20.7	1938	1920–1954	1892–1958	
β-Calacorene	16	1940.3	21.1	1933.5		1915–1984	(d); 1918 (Ref. 76); 1979 (Ref. 77)
Cubebol	32	1941.7	26.3	1957	1928–1957	1884–1964	1957 (Ref. 74); 1964 (Ref. 49)
Heptanoic acid	74	1950.9	22.6	1951	1935–1965	1916–1993	
Dendrolasin	2						1954 (Ref. 78)
p-Cresol, 2-methoxy-	24	1954.2	17.2	1956	1943–1962	1933–1980	
Jasmone, (Z)-	35	1955.2	19.5	1961	1945–1969	1914–1977	
1-Dodecanol	65	1959.3	18.7	1964	1950–1973	1924–1980	
Phenylethyl 3-methylbutanoate	11	1969.5	14.7	1964		1954–1992	
Nepetalactone, 4aα,7α,7aα	1						1970 (Ref. 79)
Piperitenone oxide	5					1940–1984	1983 (Ref. 80)
Caryophyllene oxide	297	1986.2	25.1	1987	1970–2008	1936–2023	
Phenol	141	1992.1	28.2	1997	1973–2014	1933–2032	
Methyl tetradecanoate	19	1996.2	8.8	1998		1978–2037	(d,u); 1993–2002 (Ref. 40)
4,5-Epoxy-2-decenal, (E)-	57	2000.7	12.9	2000	1993–2009	1978–2021	
Methyl eugenol	76	2006.3	24.4	2013	1986–2029	1961–2033	
Perilla alcohol	34	2006.6	21.9	2007	1991–2025	1963–2029	2016 (Ref. 49); 2029 (Ref. 74)
Nerolidol, (Z)-	22	2007.3	12.9	2006.5	1995–2017	1992–2027	
p-Anisaldehyde	36	2010.7	23.1	2009	1989–2029	1980–2050	
2-Pentadecanone	25	2015.9	12.5	2019	2010–2023	1996–2031	
α-Humulene oxide	12	2019.6	17.9	2015		1992–2083	(d)
γ-Nonalactone	82	2026.1	21.1	2024	2012–2039	1993–2063	
Carotol	7	2027.6	11.2	2024		2014–2045	(d); 2045 (Ref. 74)
Guaiacol, 4-ethyl-	59	2029.9	20.8	2032	2020–2039	1986–2065	
Furaneol	138	2031.1	19.3	2031	2020–2041	1993–2066	
Cinnamaldehyde, trans-	6	2033.2	11.5			2015–2044	
Salvial-4(14)-en-1-one	17	2035.9	5.9	2037		2016–2043	(d); 2037 (Ref. 74); 2016 (Ref. 49)
Nerolidol, (E)-	164	2036.3	19.6	2041	2027–2050	1995–2055	
Ledol	44	2039.1	17.9	2033.5	2025–2057	2014–2062	
Pentadecanal	18					1980–2060	(d); 2041 (Ref. 81); 1999 (Ref. 45)
Caryophyllenyl alcohol	2					2044–2054	
Ethyl tetradecanoate	41	2045.7	15.3	2046	2038–2055	2025–2070	
Humulene epoxide II	62	2047.3	27.2	2064	2024–2071	2003–2071	(d); 2070 (Ref. 78); 2071 (Ref. 74)
Gleenol	12					2008–2054	(d); 2051 (Ref. 82); 2051 (Ref. 45)
Germacrene-D-4-ol (Ref. 54)	29	2056.9	12.1			2000–2070	(d,v); 2069 (Ref. 83)
Octanoic acid	228	2057.1	23.9	2059	2044–2075	2011–2089	2039–2056 (Ref. 40)
Cubenol	67	2067.8	23.7	2080	2059–2080	2019–2090	
p-Cresol	98	2073.0	32.8	2080	2057–2091	2003–2121	
Cubenol, 1,10-di-epi-	5					2022–2074	2074 (Ref. 49)
Methyl cinnamate, trans-	14	2074.6	21.6	2079		2046–2105	(d)
Hexyl benzoate	21	2074.6	22.2	2074	2066–2095	2033–2097	
Elemol	88	2078.8	19.1	2080	2072–2096	2043–2103	
Sesquisabinene hydrate, cis-	2	2081.5				2075–2088	
Globulol	97	2082.4	17.3	2085	2070–2098	2049–2104	
β-Oplopenone	20	2084.5	17.4	2092	2085–2092	2049–2097	
β-Elemol	10	2087.7	11.5	2089.5		2070–2105	
1-Cubenol, epi-	23	2088				2026–2090	(d); Average of RI data (Refs. 45, 49, and 74)

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TABLE 5. Retention indices of essential oil components for polar phase—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
Guaiol	30	2088.9	14.3	2091	2080–2103	2061–2104	
Viridiflorol	102	2089.8	19.3	2093	2083–2104	2041–2110	
Sesquisabinene hydrate, trans-	3					1980–2092	
Geranyl tiglate	3	2099.3	4.9			2096–2105	
Globulol, epi-	11					2000–2100	(d); 2100 (Ref. 72)
p-Cymen-7-ol	28	2100.7	15.6	2107	2093–2113	2070–2114	
γ-Eudesmol, 10-epi-	16	2105.8	12.8	2107.5		2089–2121	
3-Hexenyl benzoate, (Z)-	31	2119.4	25.7	2122	2107–2142	2071–2148	
Cedrol	25	2119.6	18.8	2118	2102–2132	2093–2149	
Hexahydrofarnesylacetone	40	2124.8	12.1	2131	2126–2131	2096–2131	
Spathulenol	208	2126.6	22.7	2133	2117–2144	2074–2150	
Hexadecanal	19	2132.0	19.5	2135		2094–2164	
γ-Decalactone	83	2135.3	25.4	2137	2125–2151	2090–2178	
β-Copaen-4α-ol	3					2020–2141	
β-Bisabolol	12	2143.1	27.2	2143		2090–2189	(d)
Valeranone	6	2145.1	9.5	2145		2128–2155	
1-Tetradecanol	10	2152.4	16.1	2156		2123–2174	
Patchouli alcohol	4					2156–2188	
Longiborneol	6	2157.2	10.1	2154		2147–2174	
Nonanoic acid	109	2159.1	27.8	2165	2138–2178	2110–2196	
Eugenol	187	2162.7	28.1	2166	2151–2185	2100–2198	
α-Acorenol	5					2123–2207	2163 (Ref. 49)
Thymol	125	2164.3	35.7	2176	2130–2198	2100–2205	2190 (Ref. 78); 2198 (Ref. 74); 2156 (Ref. 84)
α-Cadinol, epi-	129	2169.7	19.4	2169	2156–2187	2136–2200	
γ-Eudesmol	59	2176.1	15.6	2177	2170–2185	2147–2199	
α-Muurolol	94	2183.1	27.5	2187	2165–2205	2135–2219	
Guaiacol, p-vinyl-	120	2185.6	22.2	2184	2173–2200	2145–2219	
α-Muurolol, epi-	122	2186.4	18.7	2185	2175–2209	2153–2209	
δ-Decalactone	67	2187.8	26.4	2190	2178–2205	2137–2221	
Bulnesol	16	2205.3	22.9	2201		2171–2248	(d); 2248 (Ref. 85)
β-Phenylethyl tiglate	8					2154–2227	(d)
Methyl hexadecanoate	47	2210.6	19.9	2210	2200–2223	2175–2245	
Carvacrol	139	2210.8	35.1	2223	2186–2239	2140–2246	
α-Bisabolol	56	2213.6	17.7	2213.5	2204–2232	2178–2234	
α-Bisabolol, epi-	12	2214.3	23.9	2211		2186–2256	(d); 2256 (Ref. 59)
α-Eudesmol	69	2222.7	20.6	2229	2212–2234	2186–2250	
α-Cadinol	163	2227.3	23.0	2225	2218–2255	2180–2255	
β-Sinensal	27	2229.3	21.1	2237		2186–2254	(d)
2-Heptadecanone	7	2229.7	20.1	2231		2196–2255	
Isospathulenol	8	2230.8	16.4	2231		2206–2254	(d); 2238 (Ref. 49)
Elemicin	21	2231.3	16.1	2228	2219–2245	2214–2260	
Cadalene	28					2146–2256	(d); 2256 (Ref. 57); 2233 (Ref. 45)
β-Eudesmol	128	2238.0	21.3	2239.5	2222–2256	2196–2272	
Himachalol	4	2240.8	3.8	2240		2237–2246	
Intermedeol	5	2243.0	22.2	2247		2218–2264	
Ethyl hexadecanoate	59	2249.3	17.9	2251	2238–2259	2223–2279	
Selin-11-en-4α-ol	20	2252.0	25.0	2255	2247–2273	2207–2274	
Farnesyl acetate, (2E,6E)-	16	2259.2	18.7	2260		2222–2283	
Myristicin	12	2261.4	19.9	2259		2225–2296	(d); 2296 (Ref. 86)
Eugenol acetate	4	2266.3	11.2			2252–2277	
p-Anisyl alcohol	5					2191–2290	(d); 2227–2271 (Ref. 40)
Decanoic acid	149	2273.7	23.3	2276	2261–2296	2227–2301	
Isophytol	6	2292.5	6.8	2296		2282–2299	
α-Sinensal	19	2300.8	37.2	2304		2236–2363	
Caryophylla-4(12),8(13)-dien-5α-ol	8	2301.0	19.9	2298		2272–2324	(d); 2320 (Ref. 49)
Eudesm-7(11)-en-4-ol	8					2239–2325	(d); 2320 (Ref. 83)

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TABLE 5. Retention indices of essential oil components for polar phase—Continued

Name	N (a)	Average value	Standard deviation	Median value	50% RI range	90% RI range (b)	Comment (c)
Farnesol, (2Z,6Z)-	16	2324.4	23.5	2323		2286–2355	(d,w); 2287 (Ref. 71)
Chavicol	13	2337.0	10.8	2339		2320–2358	
Farnesol, (2E,6Z)-	9					2219–2342	(w); 2341 (this work)
Dill apiole	10	2346.3	32.7			2305–2384	(d); 2384 (Ref. 61)
Farnesol, (2Z,6E)-	51	2356.8	10.6	2355	2350–2366	2340–2370	(w); 2341 (Ref. 61); 2351 (Ref. 72)
Farnesol, (2E,6E)-	6					2278–2387	(w); 2366 (this work); 2369 (Ref. 61)
Eudesma-4(15),7-dien-1β-ol	7	2371.3	11.6	2370		2351–2402	(d); 2385 (Ref. 77)
1-Hexadecanol	40	2374.9	16.3	2381.5	2365–2384	2341–2392	
Manoyl oxide	10					2335–2376	(d); 2376 (Ref. 82)
Farnesyl acetone, (5E,9E)	2					2377–2382	
Undecanoic acid	25	2390.7	24.5	2400		2339–2421	(d); 2400 (Ref. 86)
Caryophyllenol II	7					2392–2396	(t); 2392 (Ref. 74)
Methyl octadecanoate	19	2414.7	17.1	2417.5		2386–2445	
Chamazulene	9					2334–2452	(d); 2370 (Ref. 87); 2430 (Ref. 88)
Methyl oleate	10	2437.3	25.2			2400–2476	(d); 2426–2442 (Ref. 40)
Indole	38	2440.5	22.6	2444		2346–2478	(d,x)
Abietadiene	3					2449–2502	
Dodecanoic acid	96	2486.5	24.6	2489.5	2471–2503	2442–2524	
Methyl linoleate	12	2493.8	15.4	2487		2476–2523	(d)
Abietatriene	14	2506.1	18.8			2476–2530	(d); 2524 (Ref. 82)
Ethyl linoleate	18	2521.9	21.9	2522.5		2486–2573	
Nootkatone	20	2548.3	28.8	2549		2504–2595	(d)
Vanillin	109	2569.5	21.9	2569	2555–2585	2531–2605	
1-Octadecanol	15	2586.4	27.5	2598		2534–2626	(d); 2607 (Ref. 57)
Benzyl benzoate	31	2612.7	35.1	2618	2577–2648	2565–2655	(d); 2655 (Ref. 59)
Phytol	31	2613.4	12.3	2619		2510–2633	(d,y)
Tridecanoic acid	9		36.1			2573–2678	(d); 2617 (Ref. 74)
Manool	4					2370–2628	
Manool, 13-epi-	1						2676 (Ref. 89)
Tetradecanoic acid	82	2686.8	28.3	2692	2670–2713	2634–2719	
Benzyl salicylate	7	2787.5	20.5			2760–2810	(d); 2804 (Ref. 90)
Pentadecanoic acid	31					2720–2840	(d); 2822 (Ref. 74)
Hexadecanoic acid	97	2913.2	24.9	2931	2894–2931	2862–2945	
Hexadec-9-enoic acid, (Z)-	3					2888–2960	
Octadecanoic acid	7	3148.3	28.6	3137		3120–3203	(d)
Oleic acid	8					3079–3200	(d); 3200 (Ref. 91)
Linoleic acid	6					3215–3314	(d); 3290 (Ref. 91)

Comments: (a) Number of data records. (b) See (b) in Table 3. (c) See (c) in Table 3. (d) Two (or more) separate data clusters or a large data spread were observed. (e) See (e) in Table 3. (f) Mix of data for different isomers is possible. (g) Two RI data clusters. The first was deleted due to the probability of it being a misidentification (1269–1314 range). (h) See (f) in Table 3. (i) Two data clusters:1462–1482 and 1539–1541. (j) The main data cluster (with largest number of data records) was chosen to calculate the average value. (k) Average or median value in the gap between RI data clusters. (l) The main RI data cluster was used to calculate the average value. (m) The dataset possibly represents a mix of data for cis- and trans-isomers. (n) Two RI data clusters: 1583–1611 and 1650–1668. (o) Two data clusters: 1670–1680 and 1708–1740. (p) Data possibly include RI values for cis-isomer. (q) Two RI data clusters: 1668–1701 and 1738–1771. The dataset possibly represents a mix of data for trans-and cis-isomers. The calculated average corresponds to the cluster with higher retention indices; (r) Dataset possibly includes RI values for trans-isomer. (s) Two data clusters; cluster with smaller values was deleted (1628–1707). (t) Most of RI measurements belong to the group of Baser *et al.*[69] (u) Average and median RI values were calculated for the main data cluster. (v) The average RI value was calculated for data cluster with higher RI values. (w) See (i) in Table 3. (x) RI data cluster (2346–2367) was deleted for calculation of median and average values. Deleted RI values were measured on Carbowax 20M in 1980–1990. (y) Average and median RI values were calculated for the RI data cluster which includes data of Baser and Demirci. (RI = 2622).[81]

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TABLE 6. Averaged standard deviation and confidence range size for commonly reported constituents of essential oils

Stationary phase	Averaged standard deviation (iu)	Averaged 50% confidence RI range (iu)	Averaged 90% confidence RI range (iu)
Dimethylsilicone (DIMS)	8.5 (±3.7)	10.7 (±6.5)	27.1 (±12.0)
Dimethylsilicone with 5% phenyl groups (DIMS5P)	7.9 (±3.3)	6.7 (±5.3)	25.5 (±11.1)
Polyethylene glycol (PEG)	16.7 (±6.0)	22.6 (±9.7)	55.6 (±25.2)

TABLE 7. The structural assignment of four isomers of farnesol using retention data(a)

	RI (elution order)				Elution order					
Isomer	DIMS (b)	DIMS5P (b)	DIMS5P (DB5) (c)	DIMS5P (DB5) (d)	DIMS5P (XTI5) (e)	Apiezon T (f)	DIMS (OV-101) (g)	DIMS (h)	FFAP (i)	Carbowax 20M (j)
2Z,6E	1687 ± 7 (1)	1694 ± 7 (1)	1701 (1)	1722 (3)	2,3	3	3	2	3	2,3
2Z,6Z	1691 ± 2 (2)	1714 ± 6 (2)	1718 (2)	1698 (1)	1	1	1	1	1	1
2E,6E	1705 ± 11 (3)	1722 ± 6 (3)	1725 (3)	1742 (4)	4	4	4	4	4	4
2E,6Z	1710 ± 15 (4)	1744 ± 3 (4)	1746 (4)	1714 (2)	2,3	2	2	3	2	2,3

(a) DIMS—dimethylsilicone; DIMS5P—dimethylsilicone with 5% phenyl groups. (b) This work. Retention indices were estimated using the NIST GC-RI-database (see text). (c) Ref. 53. (d) Ref. 7. (e) Ref. 92. (f) Ref. 93. (g) Ref. 94. (h) Ref. 95. (i) Ref. 96. (j) Ref. 97.

4. Summary

In this work, we evaluated 505 retention indices for most frequently reported constituents of essential oils. Retention indices were evaluated for dimethylsilicone, dimethylsilicone with 5% of phenyl groups, and polyethylene glycol stationary phases and for temperature programming conditions (Tables 2–4). The data obtained cover approximately 70% to 90% of compounds typically identified in the essential oils. The data evaluation was based on the treatment of multiple measurements from the NIST GC-RI database. We analyzed data distributions of available RI measurements for components of essential oils. Particular attention was paid to cases where multimode behavior was observed.[35,36] Evaluated retention indices correspond to typically used GC measurement conditions. Data presented include average and median values along with the evaluation of confidence intervals.

The use of retention data for analytical applications has several benefits. One of the main advantages is the possibility of identifying stereo- and geometrical isomers and removing false-positive identifications. Another useful application of evaluated indices is their use for calibration purposes. Compounds from the analyzed list (Table 1) can serve as reference compounds to derive retention indices of other components instead n-alkanes. Additionally, the use of elution order data is of interest for RI data control and improvements in accuracy of retention indices and their consistency.

The set of compounds considered represents possibly the best characterized components of essential oils in terms of GC retention index measurements. The evaluated data provide information on the variability of RI measurements and, to some extent, on the accuracy in the RI determinations. This information is of interest for different procedures of chemical compound identification using GC retention indices. The derived retention data can be used for comparison purposes and to further increase the accuracy of retention index measurements.

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