Thermodynamic and Transport Properties of Carbohydrates and their Monophosphates: The Pentoses and Hexoses

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This review contains recommended values of the thermodynamic and transport properties of the five and six membered ring carbohydrates and their phosphates in both the condensed and aqueous phases. Equilibrium data, enthalpies, heat capacities, and entropies have been collected from the literature. The accuracy of these data have been assessed, adjusted to 298.15 K and to a common standard state, and entered into a catalog of thermochemical reactions. The solution of this reaction catalog yields a set of recommended values for the formation properties of these substances. The volumetric data have also been critically evaluated. Recommended values are presented for standard state molar volumes and the temperature and pressure derivatives of the molar volume, i.e., the expansivity and the compressibility. The excess property data of aqueous solutions of these substances have been correlated to yield recommended values of the parameters of the virial expansion model used to represent the data. The transport data considered here includes both viscosity and diffusion data of aqueous solutions of the carbohydrates. The available phase diagram data and transition temperatures are summarized.

Key words: carbohydrates; chemical thermodynamics; diffusion; enthalpy; entropy; evaluated data; excess properties; Gibbs energy; heat capacity; phase diagrams; viscosity; volumetric properties.

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1. Introduction

This review emerges from a research effort at the National Institute of Standards and Technology designed to provide fundamental data on processes in which biomass is enzymatically converted to useful chemicals and fuels. Data on the thermodynamic and transport properties of the five and six membered ring carbohydrates and their monophosphates in the condensed and aqueous phases play a key role in the optimization and design of both currently used and proposed industrial processes.

For many years, carbohydrates have been of interest to chemists because of their prominent and significant roles in a variety of areas. These include metabolic reactions, industrial operations yielding chemical feedstocks, and processes encountered by researchers involved in synthesis, structural elucidations, and separations. The stabilities of these compounds and their position in chemical equilibria are dictated largely by thermodynamic considerations. Because of this, we have assembled the available thermodynamic data from the literature on the five and six membered ring carbohydrates (see Fig. 1) and their monophosphates.

Earlier reviews in the literature in this area include the thermodynamic tables of Burton and et al. Without a doubt, the former pioneering review dealt only with Gibb's energy data while the latter also included enthalpy, entropy, and heat capacity data with some attention being given to partial molar properties of solutions. The extensive review of Atkinson and Morton dealt primarily with phosphorylation reactions and contained only Gibb's energy data for biochemical processes. Barman's Enzyme Handbook contains extensive references to equilibrium data for enzyme-catalyzed reactions. Enthalpies of combustion and of formation of condensed phases of organic compounds are dealt with in four excellent reviews. Domalski, Evans, and Hearing have compiled the available data on the heat capacities and entropies of organic compounds in the condensed phase. In a comprehensive paper, Angyal reviewed the available data dealing with the detailed anomeric composition of reducing sugars in solution. Most recently, Cesaro has summarized a substantial body of physicochemical data on carbohydrates. His review also contains an extensive discussion of the physical models that have been used to rationalize some features of the data.

Most of the data which have been examined in this review involve equilibrium and calorimetric measurements of the pure compounds and on their aqueous solutions. In so far as possible, we have recalculated the original data from the experimental measurements to obtain values of the thermodynamic parameters which are then entered into a catalog. This catalog serves as the basis for the solution of the thermoochemical network for these processes and substances. The least-squares solution of the network leads to a set of recommended values for both formation properties and thermoochemical parameters for specific processes.

This review also includes the transport property data for these substances and a correlation of the data leading to the excess Gibbs energy of aqueous solutions of these substances and its temperature and pressure derivatives. Information on solubilities, phase diagrams, and the pressure derivatives of the Gibbs energy is also considered. The general aim has been to provide an essentially complete coverage of the thermodynamic and transport properties of these substances. The literature is covered through 1987.

This review identifies those areas where measurements are most needed. Also, the structural similarities of the compounds can serve as a guide to estimating property data where measurements do not currently exist.

2. Conventions

2.1. Symbols, Nomenclature, Standard States, or Units

The symbols used in this review are given in the Glossary. With only a few exceptions, we have attempted to adhere to the recommendations of the International Union of Pure and Applied Chemistry (IUPAC) on symbols, nomenclature, and units. The standard states used in the construction of the tables are the same as those used in "The NIST Tables of Chemical Thermodynamic Properties". This is for a pure solid or liquid the standard state thermodynamic properties pertain to the pure substance at a pressure of 0 MPa. For aqueous solutions, the standard state for the solution is the hypothetical ideal solution at unit molality and the standard state for the solvent is the pure solvent. The thermoochemical reference temperature is 298.15 K. These standard states and reference temperature were selected prime...
Fig. 1: Open chain structural formulas of the D-aldoses and D-ketoses.
ily because of the very large existing body of thermodynamic data which is referred to it.

The notation for physical states follows that used in “The NBS Tables of Chemical Thermodynamic Properties.” It is also summarized in the Glossary.

2.2. Conventions Regarding Detailed Structural Forms

The open chain structural formulas of the D-pentoses and D-hexoses are shown in Fig. 1. The chemistry of the carbohydrates is made both complicated and interesting by the existence of different anomeric forms for each of these compounds. Thus, for each substance there exists a pure D and L form, an α and a β form, the furanose and pyranose conformers, and the open chain aldehyde and keto forms. Clearly any chemical sample of a carbohydrate may be a mixture of one or more of these forms. It will be necessary in this review to distinguish between these various forms. Also, in many cases, we do not know the specific form of the carbohydrate that was used in particular investigations. Where the investigators have provided detailed structural information for the condensed phase, we shall specify whether the compound is in the α or β form and/or in the furanose or pyranose form. In such cases, the absence of the D or L specification shall be taken to imply that the compound is the pure D or L form. The equimolar mixture of the D and L forms will be specified as “DL.” The same conventions will be adhered to for the aqueous solutions of carbohydrates except that the absence of any designation will imply that what is intended is the equilibrium mixture of the various anomers of the pure D or L form of the carbohydrate in solution.

The thermodynamic properties of the pure D and L forms are predicted by theory to be identical. The molar entropy of a mixture of D and L forms is given by:

\[ S_{DL} = S_D - R(x_D \log x_D + x_L \log x_L) \]  

Here, \( x_D \) and \( x_L \) are, respectively, the mole fractions of the D and L forms in the mixture; \( S_D \) is the molar entropy of the pure D or L form. Since the enthalpy of the DL mixture will be the same as the enthalpy of the pure D or L form, the Gibbs energy of the DL mixture is given by the following:

\[ G_{DL} = G_D + T(S_D - S_{DL}) \]  

Since the temperature and pressure derivatives of the entropy of mixing term in Eq. (1) are zero, all of the other thermodynamic properties of DL mixtures are predicted to be identical to those of the pure D or L forms.

2.3. Arrangement of Tables and of Compounds

The tables are arranged in the following general order: melting and transition temperatures, standard state volumetric properties, excess properties, transport properties, and standard state thermochemical properties. The arrangement of the compounds in the thermochemical tables follows the standard order of arrangement used in “The NBS Tables of Chemical Thermodynamic Properties.” An effort was made to have the tables reasonably self-documenting. Thus, as a rule, the tables contain references to the sources of the data, either the original or adjusted values of the data and the recommended property values.

2.4. Treatment of Uncertainties

The uncertainties associated with the recommended values of the physical properties or of the parameters of the correlating equations in Tables 1–7 were obtained in two different ways. The first method is purely statistical and assumes a normal distribution of errors with final error estimates being made at approximately 95% confidence limits. The general procedure followed when fitting data to correlating equations was to include all parameters until the standard deviation of an additional parameter became more than half the absolute value of that parameter. When these statistical methods were used, the uncertainty is given to two significant figures. The other method of assignment of uncertainties is based upon the judgment of the reviewers as to the overall reliability of the measurements. This involves both consideration of random and systematic errors. Since it frequently involves subjective judgment, error estimates obtained this way are given to only one significant figure. The reader should draw no conclusion about the relative superiority of either of these two methods of presenting uncertainties.

The uncertainties given in the reaction catalogs are assigned primarily on the basis of the evaluators’ judgment of the reliability of that particular measurement. The initial judgment may later be modified on the basis of how well that measurement fits into the solution for the entire thermochemical network. These modifications are usually kept to a minimum and the overall fit of the network is accomplished primarily by the decision of whether or not to include a particular measurement in the final network solution. When there are cross links in the thermochemical network, the residuals (observed minus calculated values) obtained from the fit are useful in assessing both the accuracy of how well a particular measurement fits into the network and, in part, the accuracy of that particular measurement. This device serves as a good test of the overall accuracy of the thermochemical data and is useful in locating possible errors in existing measurements. In the absence of either of these cross links or replicate measurements on specific process, the user should exercise caution in accepting the assigned uncertainties for an individual processes.

The uncertainties given in the calculated values of the thermochemical properties at 298.15 K (Table 15) are standard deviations and are a measure of the overall fit of the network. It is not the uncertainty to be associated with the property and it should not be used to calculate the uncertainty pertinent to a given process.

2.5 References for the Tables

The form of the references in the tables follows that used in the “CODATA Thermodynamic Tables.” Thus, the references are ordered chronologically and alphabetically by author(s) within each year using a code consisting of the final two digits of the year and the first three letters of the first two authors’ names.

3. Excess and Partial Molar Properties

The excess Gibbs energy of aqueous solutions of the hydrates is represented by a virial expansion in the molarity of the solute:

\[ G^\text{ex} = \Sigma g_i m_i^{(i+1)} \]

The symbol “i” in the above equation and in the ones below refers to the total number of parameters needed to present the experimental data over the molarity range of interest. The symbols are defined in the Glossary. Appropriate derivatives of the excess Gibbs energy lead to the following working equations for the activity and osmotic coefficients, apparent molar, and excess properties:

\[ G^\text{ex} = \Sigma g_i m_i^{(i+1)} = m^* G^\text{ex}_1 + mG^\text{ex}_2, \]

\[ G^\text{ex}_2 = \left( \frac{\partial G^\text{ex}}{\partial m} \right)_p = \Sigma (i + 1) g_i m_i, \]

\[ G^\text{ex}_1 = -\left( \frac{1}{m^*} \right) \Sigma g_i m_i^{(i+1)}, \]

\[ G^\text{id}_1 = G^\text{id}_2 + RT \log v_i, \]

\[ G^\text{id}_2 = G^\text{id}_1 + RT \log v_i = G^\text{id}_2 + RT \log v_i \]

\[ \gamma = \exp \left[ \left( \frac{G^\text{ex}_1}{(RT)} \right) \right], \]

\[ \phi = \left( \frac{m^*}{m} \right) \log v_i = \left[ m^* G^\text{ex}_1 / (mRT) \right] + 1, \]

\[ S^\text{ex} = -\left( \frac{\partial G^\text{ex}}{\partial T} \right)_p = \Sigma h_i m_i^{(i+1)}, \]

\[ S^\text{id}_1 = S^\text{id}_2 + R \log v_i \]

\[ S^\text{id}_2 = \left( \frac{\partial S^\text{id}}{\partial m} \right)_p = \Sigma (i + 1) h_i m_i \]

\[ H^\text{ex} = G^\text{ex} + T \left( \frac{\partial G^\text{ex}}{\partial T} \right)_p = \Sigma h_i m_i^{(i+1)}, \]

\[ H^\text{id}_2 = H^\text{id}_1 + RT \log v_i \]

\[ H^\text{id}_1 = C^\text{id}_1 + \frac{V_m}{m} \]

\[ L = H - H^\text{ex} = m^* / m = \Sigma h_i m_i \]

\[ L^\text{ex} = \left( \frac{\partial L^\text{ex}}{\partial m} \right)_p = \Sigma v_i m_i \]

\[ C^\text{ex}_p = \left( \frac{\partial H^\text{ex}}{\partial T} \right)_p = \Sigma c_i m_i^{(i+1)}, \]

\[ C^\text{ex}_2 = \left( \frac{\partial C^\text{ex}}{\partial m} \right)_p = \Sigma (i + 1) c_i m_i, \]

\[ C^\text{ex}_p = C^\text{ex}_2 + (C^\text{ex}_p / m) = \Sigma c_i m_i^{(i+1)}, \]

\[ c_p = (1 + mM_2)^{-1}, \]

\[ V = \left( \frac{\partial G^\text{ex}}{\partial p} \right)_T = \Sigma v_i m_i^{(i+1)}, \]

\[ V_2 = \left( \frac{\partial V^\text{ex}}{\partial m} \right)_p = \Sigma (i + 1) v_i m_i, \]

\[ V_1 = V^\text{id}_1 = V^\text{id}_1, \]

\[ M_2 = \frac{V_2}{V_1}, \]

\[ \rho = 1 + (1 + M_2) \left( \frac{V^\text{ex} / m}{V^\text{ex} / m + M_2} \right) \]

The above equations also include expressions for the ideal Gibbs energy, entropy, enthalpy, and volume. The quantities \( m^* \) and \( m \), respectively, are equal to 1 and 55.5084 mol kg\(^{-1}\). The former quantity is introduced to preserve the dimensionality of units, and the latter is the amount of water in a kilogram of water. The use of excess and apparent molar properties offers a concise and convenient way of representing the results of a large variety of physical property data. Note that the excess Gibbs energy is not a molar Gibbs energy; it has units of J kg\(^{-1}\). The excess Gibbs energy is obtained primarily from both direct and relative (isopiestic) vapor pressure measurements, the excess enthalpy from heats of dilution, and the excess heat capacity from direct heat capacity measurements on aqueous solutions. The excess volume and expansivity are obtained from precise density measurements, the latter quantity requiring that the densities be determined as a function of temperature. The isothermal compressibility is rarely measured. However, the isentropic compressibility is conveniently determined from measurements of the speed of sound (\( a \)) and a knowledge of the density (\( \rho \)):

\[ \kappa_S = V^{-1} \left( \frac{\partial V}{\partial p} \right)_S = K_S / V = 1 / (\rho a^2). \]

The isothermal compressibility is then calculated using the following relationship:

\[ K_T^\text{o} = K_T^\text{o} + 2(\kappa_T^\text{o} - \kappa_S^\text{o}) \]

\[ \times \left[ \left( \frac{V_{\text{ex}}}{V_{\text{ex}}} \right) / E_{\text{ex}} \right] \left[ \frac{C_p^\text{o} - V_{\text{ex}}}{C_p^\text{o}} \right] \]

4. Sources of Auxiliary Data

The sources for the values of the fundamental physical constants and atomic masses used in this review are, respectively, the 1986 Committee on Data for Science and Technology (CODATA)\( \text{16} \) and the 1981 IUPAC recommendations.\( \text{17} \) Auxiliary thermochemical data (see Table 1) were taken primarily from the most recent set of CODATA recommended values.\( \text{18} \) The properties of \( \text{Na}^+ \) and \( \text{Cl}^– \) are those given in “The NBS Tables of Chemical Thermodynamic Properties”.\( \text{19} \) The partial molar heat capacities of \( \text{HPO}_4^{2–} \) (aq) and of \( \text{H}_2\text{PO}_4 \) (aq) are from Larson, Zeeb, and Hepler.\( \text{20} \) The partial molar heat capacities of \( \text{Mg}^{2+} \) (aq) and \( \text{Ca}^{2+} \) (aq) are from Spitzer, Olofsson, Singh, and...
Hepler.\textsuperscript{23} Except for the entropy and the Gibbs energy and enthalpy of formation, the properties of pure water were taken from the "NBS/NRC Steam Tables".\textsuperscript{24}

5. Contents and Descriptions of the Tables

Tables 1–3 contain data on the transition temperatures and volumetric properties of the pure carbohydrates in condensed phases. Note that many of the densities were calculated using the results of crystallographic studies.\textsuperscript{25} All of the crystalline carbohydrates considered in this review are orthorhombic with four molecules per unit cell and fall into space group $2_12_12_1$. There is a very limited amount of data available on the cubic expansion coefficients of these carbohydrates in condensed phases and no information on their compressibilities.

The available phase diagram data are shown in Figs. 2 and 3 and are based primarily upon careful work done at the National Bureau of Standards over 60 years ago.\textsuperscript{26,27} Glucose exists as both a monohydrate and in the anhydrous form with the transition occurring at 323.15 K. The phase diagram for fructose is more complex and shows the existence of a gel, the anhydrous compound, a metastable crystalline phase, a dihydrate, and a hemihydrate.

The standard state volumetric data from the literature on aqueous carbohydrates are given in Table 4. The recommended values of the standard state partial molar volumes, expansivity, isentropic and isothermal compressibility, and the temperature derivative of the isentropic compressibility are given in Table 5. In computing isothermal compressibilities from the isentropic compressibilities, the needed value of $C_P^0$ were taken from Table 15 of this paper. The extremely precise and careful measurements of Bernal and van Hook\textsuperscript{45} on aqueous glucose and fructose are preferred over the earlier data.

Table 6 contains values of the parameters of the correlating equations (see Sec. 3 above) of the excess Gibbs energy, enthalpy, heat capacity, volume, expansivity, and the isentropic compressibility and its temperature derivative. In nearly all cases the correlations are based upon the results of a single investigation, the exceptions being the data leading to the excess Gibbs energy and enthalpy of aqueous glucose solutions. For the excess Gibbs energy the most weight has been given to the isopiestic data of Stokes and Robinson\textsuperscript{9} and of Miyajima, Sawada, and Nakagi.\textsuperscript{30} The results of Taylor and Rowlinson\textsuperscript{31} are based upon direct vapor pressure measurements. This method of measurement is more difficult than the isopiestic approach, and typically yields results that are less accurate. A deviation plot of observed and calculated values of the osmotic coefficient of aqueous glucose solutions as a function of the molality is shown in Fig. 4. The heat of dilution data of aqueous glucose solutions determined by Lange and Markgraf\textsuperscript{32} and by Savage and Wood\textsuperscript{33,34} are in excellent agreement with each other. Plots of the excess Gibbs energy, enthalpy, and entropy are shown in Figs. 5–7. Note that in all cases the excess Gibbs energy, entropies, and enthalpies are positive and that the entropic contributions ($T \Delta S^\circ$) to the excess Gibbs energies are negligible.
Deviations plot (observed minus calculated values) of the osmotic coefficient of aqueous glucose solutions as a function of the molality. The data sets are from the following sources: (△) Taylor and Rowlinson (Ref. 31), (□) Bonner and Breazeale (Ref. 29a), (○) Stokes and Robinson (Ref. 29), (+) Miyajima et al. (Ref. 30), NaCl reference solution and (×) Miyajima et al. (Ref. 30), CaCl₂ reference solution.

A substantial proportion (30-70%) of the enthalpic contributions.

There is a very limited amount of transport property data available on aqueous carbohydrate solutions. It is summarized in Table 7.

Table 8 contains the percent composition of the anomic forms of the hexoses and pentoses taken from the thorough review of Angyal. Using these data and the few estimates given in Table 9, the Gibbs energy changes at 298.15 K for the conversion of the various anomic forms to the equilibrium mixture have been calculated. The results of these calculations are given in Table 9. In the main body of the thermochemical tables (Tables 11–15) only the equilibrium mixture of the anomic forms of the carbohydrates is considered. Thus, Gibbs energy changes for processes involving specific anomic forms of the carbohydrates can be calculated using an appropriate combination of the Gibbs energy.
changes in Table 9 with the Gibbs energy data contained in Tables 11–15. There is also a limited amount of information available on enthalpy, heat capacity, and volume changes involving specific anomeric forms of the carbohydrates. It is summarized in Table 10. Note that there is a large enthalpy difference between the pyranose and furanose forms of fructose. However, the enthalpy differences between the α and β forms of the carbohydrates are relatively small and the entropy differences between these forms are close to zero.

Table 11 contains the reaction catalog of Gibbs energy, enthalpy, and entropy data pertinent to these carbohydrates and their monophosphates; the heat capacity catalog is given in Table 12. The indexes of compounds and their reactions in reference to these two catalogs are given in Tables 13 and 14, respectively. These indexes are useful in examining cross links between the data for specific compounds and reactions. Table 15 contains the calculated values of the thermochemical properties at 298.15 K with the auxiliary thermochromic data used being given at the end of the table. The reaction catalogs are in similar format to those given in the "CO-DATA Thermodynamic Tables" and in the review by Parker, Evans, and Nuttall in rubidium compounds. Note that compounds having the same empirical formula are distinguished in the Tables 12–15 by the addition of a number to the abbreviation designating the physical state of the substance. The molar masses used in these tables are based upon the 1981 Atomic Weights; the mass of the electron is considered when calculating molar masses of charged species.

In the thermochemical tables, the experimental data reported in individual papers have been adjusted, insofar as possible, to 298.15 K and to the thermochemical standard state (see Sec. 2.1). These adjustments have frequently required the use of estimated enthalpies and/or heat capacities, activity coefficients, and equilibrium modeling calculations to obtain the thermochemical parameters for appropriate reference reactions at 298.15 K and at the standard state. In the absence of direct measurements, it has frequently been necessary to estimate activity coefficients. This has usually been done using an extended Debye–Hückel expression with the B or "ion size" parameter set equal to 1.6 mol^{-1/2} kg^{-1/2}.

In constructing the thermochemical tables it was necessary to make estimates of two of these properties, specifically the partial molar entropies of aqueous ribose and ribose 5-phosphate. The estimated entropy of 204 ± 20 J mol^{-1} K^{-1} for aqueous ribose is based upon the partial molar entropy of aqueous xylose. In this respect, note that the values of the partial molar entropies of the aqueous hexoses are reasonably close to each other. The estimated entropy of 69 J mol^{-1} K^{-1} for aqueous ribose 5-phosphate is based upon an experimental determination of the enthalpy change (−5.69 kJ mol^{-1}) and an estimated equilibrium constant of 420 for the hydrolysis of ribose 5-phosphate. Since these two estimates substantially extend the thermochemical network, we believe that they are useful. Clearly, measurements which would eliminate the need for these estimates would be desirable.

6. Trends and Physical Interpretation of the Data

6.1. Ranges of Property Values

Table 16 contains the range of values for many of the properties considered in this review. Among the most usef...
Thermodynamic and Transport Properties of Carbohydrates

H. H. Cole and A. H. K. Somsen\textsuperscript{42,43} used both preferential solvation and hydrophobic hydration arguments to account for enthalpies of transfer of carbohydrates from water to \textit{N},\textit{N}-dimethylformamide solutions.

An alternative approach for the representation of these properties has been proposed by Savage and Wood.\textsuperscript{23} They assumed that each functional group in a molecule interacts with every functional group in the other molecule so that this interaction is independent of the positions of functional groups in the two molecules. Each interaction has a characteristic effect on the excess property. These interaction energies are regressed from a body of experimental data and can be used to predict properties of additional systems which have not yet been measured. Barone and co-workers\textsuperscript{44} have applied this approach to the excess properties of aqueous carbohydrate solutions. They have also attempted to correlate the property differences between the sugars with differences in stereochemistry.

Bernal and van Hooij\textsuperscript{45} have summarized several attempts at property data rationalization which involved structure making and breaking effects. They concluded that attempts along this line had not been successful. They also made the useful observation that the “volumetric properties of carbohydrates are similar in sign if not in magnitude to those commonly associated with strong electrolytes.”

The problem of the rationalization of properties of systems of the type considered here is a particularly difficult one, presently, unresolved issue. The systematic collection and evaluation of additional property data would significantly aid progress in this area. This data can then be carefully examined either to suggest or substantiate improved physical models for these systems.

7. Needed Measurements

Examination of the data in the tables can also serve to guide the selection of new measurements. In certain areas, the data is particularly sparse, e.g., transport properties and phase diagrams. Additional data in these areas should prove helpful. While the equilibrium or Gibbs energy data relating different anomeric forms of the carbohydrates is reasonably good, there is relatively little information available on enthalpy, heat capacity, or volume changes in this field. An area of excess property data the enthalpies are the most complete in terms of available data. Thus, we would like to see additional isosteric measurements performed on aqueous sugar and sugar phosphate solutions. There is a real need for the measurements of heat capacities of solutions as a function of molality. This would permit the accurate calculation of the virial parameters of the excess heat capacity. Amination of the heat capacity catalog (Table 12) shows several discrepancies which need to be resolved. Here, the a for aqueous fructose is the prime example. Also, there are no direct heat capacity measurements on aqueous solutions of the sugar phosphates.

All of the third law entropies contained in the thermocatalytic tables involved long extrapolations to the absolute zero of temperature and, therefore, have larger uncertainties than can be obtained using modern methods. In particular, would welcome third law entropies determined on another numerically well characterized samples of crystalline glucose, fructose, ribose, and xylose. An understanding of how the various anomeric forms differ in their third law entropies would be extremely interesting. Similarly, the discrepancies in several of the enthalpies of combustion, mannose and fructose in particular, need to be resolved. In constructing the thermochemical catalog we were able to obtain a very tight and consistent solution of the network involving the aqueous solute species by giving zero weight to those reactions involving ATP (adenosine 3′,5′-diphosphate) coupled processes. Therefore, the residuals in these latter processes are larger than their assigned uncertainties. We suspect that these discrepancies are due either to (i) unsuspected side reactions or (ii) to the proton and metal-ion binding corrections, or (iii) to the adjustment to the thermochemical standard state. In any case the uncertainties in the Gibbs energies and enthalpies of ATP coupled processes (reactions 105–110) are larger than initially believed. Further attention in this area is needed. The thermochemical network also used two estimated entropies, specifically for aqueous ribose and ribose 5-phosphate (see Sec. 5 above). The former estimate could be made redundant if a third law entropy were determined for ribose (cr). The preferred pathway for eliminating the second estimate involves a determination of the equilibrium constant for the hydrolysis of ribose 5-phosphate to ribose and inorganic phosphate. This data could then be combined with the enthalpy change for this reaction and the partial molar entropy of aqueous ribose determined from a third law entropy of the crystal. Examination of the thermochemical network also indicates the need for additional measurements on other enzyme-catalyzed reactions. Specifically, we would like to see equilibrium data determined for the hydrolyses of ribulose 5-phosphate and ribose 1-phosphate and direct calorimetric measurements performed on the isomerizations of glucose 1-phosphate to glucose 6-phosphate, of galactose 1-phosphate to glucose 1-phosphate, and of aqueous mannose to fructose. An error in the enthalpy change for this latter process could help to explain the discrepancies in the enthalpies of combustion of crystalline mannose and fructose.

The thermodynamic data contained in these tables is useful both for examining efficiencies and for optimizing the reaction conditions for industrially useful processes. For example, the data contained in these tables can be used to calculate the temperature dependency of the conversion of glucose to fructose.\textsuperscript{44} Similarly, there is substantial interest in the production of ethanol from biomass.\textsuperscript{47,48} The formation properties given in Table 15 together with those for ethanol\textsuperscript{44} can be used to examine the efficiencies of proposed processes in this area. In summary, the thermochemical catalog approach is useful for examining the consistency of thermodynamic data and in expanding its predictions. We would like to see it extended to other networks involving enzyme-catalyzed reactions and to biochemical processes in general.

8. Acknowledgments

We thank Dr. David Garvin, Dr. Ralph Nuttall, and Mrs. Dorothy Bickham for their help with the computer program used to obtain a solution of the thermochemical

9. References in the Text


### TABLE 1. Melting and transition temperatures of the pure carbohydrates.

Unless indicated otherwise, the data were taken from [42BAT]

<table>
<thead>
<tr>
<th>Carbohydrate</th>
<th>Melting or transition temperature °C</th>
</tr>
</thead>
<tbody>
<tr>
<td>β-arabinose</td>
<td>160</td>
</tr>
<tr>
<td>lyxose:</td>
<td></td>
</tr>
<tr>
<td>α form</td>
<td>106–107</td>
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<tr>
<td>β form</td>
<td>117–118</td>
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<td>β-altrose</td>
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<td>α-galactose:</td>
<td></td>
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<td>167</td>
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<td>hydrate</td>
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<tr>
<td>α form</td>
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<tr>
<td>α monohydrate</td>
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<tr>
<td>β form</td>
<td>148–150</td>
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<tr>
<td>gulose</td>
<td>syrup</td>
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<td>idose</td>
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<td>mannose:</td>
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<tr>
<td>α form</td>
<td>133</td>
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<tr>
<td>β form</td>
<td>132</td>
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<tr>
<td>psicose</td>
<td>syrup</td>
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<td>sorbose</td>
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<tr>
<td>tagatose</td>
<td>134–135°</td>
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<td>talose:</td>
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<tr>
<td>α form</td>
<td>133–134</td>
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<tr>
<td>β form</td>
<td>120–121</td>
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</tbody>
</table>

*Transition temperature of dihydrate to anhydrous [52YOU/JON].
*Data from compilation of [82BAI].
*Transition temperature of monohydrate to anhydrous [22JAC/SIL].
TABLE 2. Densities and cubic expansion coefficients of the pure carbohydrates near 298 K obtained from the literature

<table>
<thead>
<tr>
<th>Carbohydrate</th>
<th>( \rho ) g cm(^{-3})</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \beta )-D-allose</td>
<td>1.593(^a)</td>
<td>[84KRO/SLU]</td>
</tr>
<tr>
<td>( \beta )-arabinose</td>
<td>1.619(^a)</td>
<td>[61HOR]</td>
</tr>
<tr>
<td>( \beta )-L-arabinose</td>
<td>1.626(^b)</td>
<td>[77TAK/JEF]</td>
</tr>
<tr>
<td>( \beta )-D-l-arabinose</td>
<td>1.636(^b)</td>
<td>[67KIM/JEF]</td>
</tr>
<tr>
<td>( \beta )-D-fructose</td>
<td>1.640(^b)</td>
<td>[79TAK/NOR]</td>
</tr>
<tr>
<td>( \beta )-D-fructopyranose</td>
<td>1.601(^b)</td>
<td>[77KAN/ROE]</td>
</tr>
<tr>
<td>( \alpha )-D-galactose</td>
<td>1.615(^b)</td>
<td>[76OHA/GIL](^d)</td>
</tr>
<tr>
<td>( \alpha )-D-galactose</td>
<td>1.611(^b)</td>
<td>[76SHE]</td>
</tr>
<tr>
<td>( \alpha )-D-galactose</td>
<td>1.579(^b)</td>
<td>[75LUJ/UEH](^a)</td>
</tr>
<tr>
<td>( \alpha )-D-galactose</td>
<td>1.595(^b)</td>
<td>[76SHE]</td>
</tr>
<tr>
<td>glucose (glass)</td>
<td>1.523(^b)</td>
<td>[82PAR/HUF]</td>
</tr>
<tr>
<td>glucose (cr)</td>
<td>1.540(^b)</td>
<td>[66KAM/UGG]</td>
</tr>
<tr>
<td>( \alpha )-D-glucose</td>
<td>1.566(^a)</td>
<td>[65BRO/LEV]</td>
</tr>
<tr>
<td>( \alpha )-D-glucose</td>
<td>1.560(^a)</td>
<td>[74SWA/MUR]</td>
</tr>
<tr>
<td>( \rho )-D-glucose (cr)</td>
<td>1.562(^a)</td>
<td>[79BRO/LEV]</td>
</tr>
<tr>
<td>lyxose (cr)</td>
<td>1.544(^a)</td>
<td>[66HOR]</td>
</tr>
<tr>
<td>( \beta )-L-lyxopyranose (cr)</td>
<td>1.536(^a)</td>
<td>[78NOR/TAK]</td>
</tr>
<tr>
<td>mannose (cr)</td>
<td>1.501(^b)</td>
<td>[31MAR]</td>
</tr>
<tr>
<td>( \alpha )-D-mannopyranose (cr)</td>
<td>1.564(^b)</td>
<td>[76LON/AVE]</td>
</tr>
<tr>
<td>D-ribose (cr)</td>
<td>1.591(^a)</td>
<td>[56FUK/HOR]</td>
</tr>
<tr>
<td>( \alpha )-L-sorbopyranose (cr)</td>
<td>1.607(^b)</td>
<td>[67KIM/RYS]</td>
</tr>
<tr>
<td>( \alpha )-L-sorbopyranose (cr)</td>
<td>1.602(^b)</td>
<td>[79NOR/TAK]</td>
</tr>
<tr>
<td>( \alpha )-D-tagatose (cr)</td>
<td>1.655(^c)</td>
<td>[69TAK/RYS]</td>
</tr>
<tr>
<td>( \alpha )-D-talose (cr)</td>
<td>1.591(^b)</td>
<td>[77HAN/HOR]</td>
</tr>
<tr>
<td>( \alpha )-D-talopyranose (cr)</td>
<td>1.602(^b)</td>
<td>[77OHE/AVE]</td>
</tr>
<tr>
<td>D-xyllose (cr)</td>
<td>1.617(^a)</td>
<td>[58WOO]</td>
</tr>
<tr>
<td>( \alpha )-L-xyllypyranose (cr)</td>
<td>1.511(^c)</td>
<td>[71HOR]</td>
</tr>
<tr>
<td>( \alpha )-L-xyllypyranose (cr)</td>
<td>1.663(^b)</td>
<td>[80JEF/ROB]</td>
</tr>
<tr>
<td></td>
<td>1.524(^b)</td>
<td>[79TAK/NOR]</td>
</tr>
</tbody>
</table>

Cubic expansion coefficients at 298.15 K

<table>
<thead>
<tr>
<th>Compound</th>
<th>( \alpha \times 10^4 ) K(^{-1})</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>glucose (cr)</td>
<td>3.1</td>
<td>[82PAR/HUF]</td>
</tr>
<tr>
<td>glucose (glass)</td>
<td>2.4</td>
<td>[65RAM/GOR](^d)</td>
</tr>
</tbody>
</table>

\(^a\) One set of x-ray data for \( \alpha \)-L-xyllypyranose was determined at 123 K by [80JEF/ROB].

\(^b\) Determined by flotation method.

\(^c\) Calculated from x-ray data.

\(^d\) [65RAM/GOR] report the existence of a second order phase transition at \( \approx 296.2 \) K. Below this temperature, the cubic expansion coefficient is equal to \( 5.1 \times 10^{-4} \) K\(^{-1}\).
<table>
<thead>
<tr>
<th>Hydrolylate</th>
<th>(\rho \times 10^{3}) g cm(^{-3})</th>
<th>(V' \times 10^{4}) m(^{3}) mol(^{-1})</th>
<th>(\alpha' \times 10^{4}) K(^{-1})</th>
<th>(E' \times 10^{4}) m(^{3}) mol(^{-1}) K(^{-1})</th>
</tr>
</thead>
<tbody>
<tr>
<td>* (\alpha)-cellucrose(cr)</td>
<td>1.593±0.005</td>
<td>113.1±0.4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>* (\alpha)-allose(cr)</td>
<td>1.624±0.01</td>
<td>92.44±0.6</td>
<td></td>
<td></td>
</tr>
<tr>
<td>* (\alpha)-arabinose(cR)</td>
<td>1.638±0.005</td>
<td>91.65±0.3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>* (\beta)-treose(cR)</td>
<td>1.600±0.005</td>
<td>112.6±0.4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>* (\beta)-nosacyranose(cR)</td>
<td>1.599±0.005</td>
<td>112.7±0.4</td>
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<td></td>
</tr>
<tr>
<td>* (\gamma)-galactose(cR)</td>
<td>1.619±0.005</td>
<td>111.3±0.4</td>
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<td></td>
</tr>
<tr>
<td>* (\delta)-galactose(cR)</td>
<td>1.587±0.01</td>
<td>113.5±0.7</td>
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</tr>
<tr>
<td>* (\alpha)-mucose(glass)</td>
<td>1.523±0.005</td>
<td>118.3±0.4</td>
<td>3.1±0.2</td>
<td>3.7±0.2</td>
</tr>
<tr>
<td>* (\alpha)-glucose(cR)</td>
<td>1.562±0.003</td>
<td>115.3±0.2</td>
<td>2.4±0.1</td>
<td>2.8±0.1</td>
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<tr>
<td>* (\beta)-glucose(cR)</td>
<td>1.552±0.005</td>
<td>116.1±0.4</td>
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<tr>
<td>* (\alpha)-cellobiose(cR)</td>
<td>1.544±0.01</td>
<td>97.23±0.6</td>
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<tr>
<td>* (\alpha)-xylopyranose(cR)</td>
<td>1.536±0.005</td>
<td>97.74±0.3</td>
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<tr>
<td>* (\alpha)-manno(cR)</td>
<td>1.501±0.01</td>
<td>120.0±0.8</td>
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<tr>
<td>* (\alpha)-mannopyranose(cR)</td>
<td>1.564±0.01</td>
<td>115.2±0.8</td>
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<tr>
<td>* (\alpha)-cello(cR)</td>
<td>1.59±0.02</td>
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<td>1.600±0.005</td>
<td>112.2±0.3</td>
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<tr>
<td>* (\alpha)-tagatose(cR)</td>
<td>1.655±0.01</td>
<td>108.9±0.7</td>
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<tr>
<td>* (\alpha)-talose(cR)</td>
<td>1.591±0.005</td>
<td>113.2±0.4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>* (\alpha)-talopyranose(cR)</td>
<td>1.602±0.005</td>
<td>112.5±0.4</td>
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<tr>
<td>* (\alpha)-xyllose(cR)</td>
<td>1.513±0.01</td>
<td>99.36±0.7</td>
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<tr>
<td>* (\alpha)-xylopyranose(cR)</td>
<td>1.524±0.01</td>
<td>98.51±0.7</td>
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</table>
Table 4. Values of standard state volumetric properties of aqueous carbohydrates at 298.15 K from the literature

<table>
<thead>
<tr>
<th>Compound</th>
<th>&quot;Best&quot; value</th>
<th>25RIB/ESP</th>
<th>26RIB/MIN</th>
<th>58SHI</th>
<th>69LED/UED</th>
<th>70NEA/GOR</th>
<th>72FRA/RAV</th>
<th>75SHA/FAL</th>
<th>77SAV</th>
<th>81HOL/HOL</th>
<th>78LOS/SHI</th>
<th>82JAS/AHL</th>
<th>83MIY/SAW</th>
<th>84JAS/AHL</th>
<th>85UED/ED</th>
<th>86BER/HOO</th>
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</thead>
<tbody>
<tr>
<td>arabinose</td>
<td>93.7±0.3</td>
<td>94.0</td>
<td>91.9</td>
<td>93.2</td>
<td>94.0</td>
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<tr>
<td>fructose</td>
<td>10.7±0.1</td>
<td>110.5</td>
<td>110.4</td>
<td>110.9</td>
<td>110.6</td>
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<tr>
<td>galactose</td>
<td>10.5±0.3</td>
<td>110.2</td>
<td>110.7</td>
<td>111.9</td>
<td>110.2</td>
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<tr>
<td>glucose</td>
<td>112.0±0.1</td>
<td>111.5</td>
<td>112.2</td>
<td>111.9</td>
<td>112.2</td>
<td>112.2</td>
<td>112.04</td>
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<td>111.99</td>
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<tr>
<td>mannose</td>
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<tr>
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<td>95.2±0.1</td>
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<td></td>
<td></td>
<td>95.5</td>
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</tr>
<tr>
<td>sorbose</td>
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<tr>
<td>ryllose</td>
<td>95.4±0.3</td>
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</tr>
</tbody>
</table>

*Adjusted from 293.15 K using values of $E_i^*$ given in Table 4.

*Data determined at 273.15 K and adjusted to 298.15 K using estimated value of $E_i^*$. 
TABLE 4. Values of standard state volumetric properties of aqueous carbohydrates at 298.15 K from the literature — Continued

Standard state partial molar expansivities \(E^*_s = E^*_e = (\partial V/\partial T)_p\). The units are \(10^{-6} \text{ m}^3 \text{ mol}^{-1} \text{ K}^{-1}\).

<table>
<thead>
<tr>
<th>Compound</th>
<th>&quot;Best&quot; value</th>
<th>70NEA/GOR</th>
<th>72FRA/RAV</th>
<th>77SAV</th>
<th>83MIY/SAW2</th>
<th>86BER/HOO</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\alpha)</td>
<td>0.136±0.01</td>
<td>0.15</td>
<td>0.15</td>
<td></td>
<td>0.11</td>
<td>0.091</td>
</tr>
<tr>
<td>(\beta)</td>
<td>0.091±0.01</td>
<td>0.10</td>
<td>0.12</td>
<td>0.11</td>
<td>0.11</td>
<td>0.15</td>
</tr>
<tr>
<td>(\epsilon)</td>
<td>0.12±0.03</td>
<td></td>
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<td></td>
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</tr>
</tbody>
</table>

Standard state partial molar isentropic compressibilities \(K^*_s = K^*_e = (\partial V/\partial T)_S\). The units are \(10^{-15} \text{ m}^3 \text{ mol}^{-1} \text{ Pa}^{-1}\).

<table>
<thead>
<tr>
<th>Compound</th>
<th>&quot;Best&quot; value</th>
<th>58SHI</th>
<th>72FRA/RAV</th>
<th>78HOL/HOL</th>
<th>78LOS/SHI</th>
<th>86BER/HOO</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\alpha)</td>
<td>-19.3±0.1</td>
<td>-14.5</td>
<td>-19.3</td>
<td></td>
<td></td>
<td>-21.37</td>
</tr>
<tr>
<td>(\beta)</td>
<td>-21.37±0.02</td>
<td>-16.5</td>
<td>-20.8</td>
<td>-17.8</td>
<td>17.50</td>
<td>17.80</td>
</tr>
<tr>
<td>(\epsilon)</td>
<td>-20.8±0.1</td>
<td>-12.8</td>
<td>-16.0</td>
<td>-16.0</td>
<td>12.5</td>
<td>12.46</td>
</tr>
<tr>
<td>(\alpha)</td>
<td>-16.0±0.1</td>
<td>-13.0</td>
<td>-12.5</td>
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<td></td>
</tr>
<tr>
<td>(\beta)</td>
<td>-12.5±0.1</td>
<td>-9.4</td>
<td>-12.9</td>
<td></td>
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<td></td>
</tr>
</tbody>
</table>

Values of the temperature derivative of the standard state partial molar isentropic compressibilities \(\left(\partial K^*_s/\partial T\right)_p\). The units are \(10^{-12} \text{ m}^3 \text{ mol}^{-1} \text{ Pa}^{-1} \text{ K}^{-1}\).

<table>
<thead>
<tr>
<th>Compound</th>
<th>&quot;Best&quot; value</th>
<th>72FRA/RAV</th>
<th>86BER/HOO</th>
</tr>
</thead>
<tbody>
<tr>
<td>fructose</td>
<td>0.80±0.1</td>
<td>1.03</td>
<td>0.80</td>
</tr>
<tr>
<td>glucose</td>
<td>0.64±0.1</td>
<td>1.14</td>
<td>0.64</td>
</tr>
</tbody>
</table>

Table 5. Recommended values of the standard state volumetric properties of aqueous carbohydrates at 298.15 K

| Compound | $V_1 \times 10^6$ m$^3$ mol$^{-1}$ | $E_T \times 10^6$ m$^3$ mol$^{-1}$ K$^{-1}$ | $K_T \times 10^{15}$ m$^3$ mol$^{-1}$ Pa$^{-1}$ | $\zeta (K_T / \alpha T) \times 10^4$ m$^3$ mol$^{-1}$ Pa$^{-1}$ K
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>arabinose</td>
<td>93.7±0.3</td>
<td>-19.3±0.1</td>
<td>-15.2±0.2</td>
<td>0.80±0.1</td>
</tr>
<tr>
<td>fructose</td>
<td>110.7±0.1</td>
<td>0.136±0.01</td>
<td>-21.37±0.02</td>
<td>0.87±0.14</td>
</tr>
<tr>
<td>galactose</td>
<td>110.5±0.3</td>
<td>0.15±0.03</td>
<td>-20.8±0.1</td>
<td>0.64±0.1</td>
</tr>
<tr>
<td>glucose</td>
<td>112.0±0.1</td>
<td>0.091±0.01</td>
<td>-17.80±0.02</td>
<td>0.64±0.1</td>
</tr>
<tr>
<td>lyxose</td>
<td>95.7±0.3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>mannosel</td>
<td>111.5±0.3</td>
<td>-16.0±0.1</td>
<td>-12.7±0.2</td>
<td></td>
</tr>
<tr>
<td>ribose</td>
<td>95.2±0.1</td>
<td>0.12±0.03</td>
<td>-12.5±0.1</td>
<td>-8.4±0.2</td>
</tr>
<tr>
<td>sorbose</td>
<td>111.0±0.3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>xylose</td>
<td>95.4±0.3</td>
<td>-12.9±0.1</td>
<td>-8.8±0.2</td>
<td></td>
</tr>
</tbody>
</table>

Table 6. Recommended values of the parameters of the correlating equations of the excess properties of aqueous carbohydrate solutions at 298.15 K. In each case the maximum molalities to which the parameters are valid are given in the next to last column.

**Parameters of the excess Gibbs energy. The units of the parameters are J kg$^{-1}$ mol$^{-1}$ (i+1)**

<table>
<thead>
<tr>
<th>Compound</th>
<th>$\varphi_1$</th>
<th>$\varphi_2$</th>
<th>$\varphi_3$</th>
<th>$\varphi_4$</th>
<th>$\varphi_5$</th>
<th>$m_{max}$ mol kg$^{-1}$</th>
<th>Workers</th>
</tr>
</thead>
<tbody>
<tr>
<td>galactose</td>
<td>-129.678±40.2</td>
<td>140.352±47.0</td>
<td>-37.884±21.0</td>
<td>3.693±2.0</td>
<td>10.00</td>
<td>$[83\text{MIY}/\text{SAW}]$</td>
<td></td>
</tr>
<tr>
<td>glucose</td>
<td>63.102±21.0</td>
<td>27.543±9.5</td>
<td>-4.084±1.5</td>
<td>0.183±0.081</td>
<td>3.45</td>
<td>$[55\text{STAY/ROW}], [65\text{BER/BER}], [66\text{STO/ROB}], [83\text{MIY}/\text{SAW}]$</td>
<td></td>
</tr>
<tr>
<td>mannosel</td>
<td>-46.678±20.0</td>
<td>68.112±19.0</td>
<td>-18.062±7.3</td>
<td>2.369±1.2</td>
<td>6.74</td>
<td>$[83\text{MIY}/\text{SAW}]$</td>
<td></td>
</tr>
<tr>
<td>ribose</td>
<td>7.501±1.6</td>
<td>3.6</td>
<td></td>
<td></td>
<td>3.66</td>
<td>$[83\text{UED}/\text{UDL}]$</td>
<td></td>
</tr>
<tr>
<td>xylose</td>
<td>81.523±3.6</td>
<td>3.6</td>
<td></td>
<td></td>
<td>3.47</td>
<td>$[89\text{UED}/\text{UDL}]$</td>
<td></td>
</tr>
</tbody>
</table>

**Parameters of the excess enthalpy. The units of the parameters are J kg$^{-1}$ mol$^{-1}$ (i+1)**

<table>
<thead>
<tr>
<th>Compound</th>
<th>$h_1$</th>
<th>$h_2$</th>
<th>$m_{max}$ mol kg$^{-1}$</th>
<th>Worker(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>arabinose</td>
<td>177.8±20.</td>
<td>7.42±5.3</td>
<td>1.61</td>
<td>$[82\text{BAR/CAC}]$</td>
</tr>
<tr>
<td>fructose</td>
<td>264.2±19.</td>
<td>-7.15±4.2</td>
<td>4.54</td>
<td>$[81\text{BAR/CAS}]$</td>
</tr>
<tr>
<td>galactose</td>
<td>132.5±8.0</td>
<td>2.01</td>
<td>2.00</td>
<td>$[81\text{BAR/CAC}]$</td>
</tr>
<tr>
<td>glucose</td>
<td>342.±10.</td>
<td>-12.4±4.0</td>
<td>2.00</td>
<td>$[82\text{BAR/CAC}]$</td>
</tr>
<tr>
<td>lyxose</td>
<td>242.7±7.5</td>
<td>-10.7±3.9</td>
<td>1.69</td>
<td>$[83\text{BAR/CAS}]$</td>
</tr>
<tr>
<td>mannosel</td>
<td>207.2±17.</td>
<td>-14.0±5.2</td>
<td>2.26</td>
<td>$[81\text{BAR/CAC}]$</td>
</tr>
<tr>
<td>ribose</td>
<td>201.7±9.1</td>
<td>-5.5±5.7</td>
<td>1.41</td>
<td>$[83\text{BAR/CAS}]$</td>
</tr>
<tr>
<td>sorbose</td>
<td>394.9±12.</td>
<td>-16.2±6.0</td>
<td>1.96</td>
<td>$[82\text{BAR/CAC}]$</td>
</tr>
<tr>
<td>xylose</td>
<td>339.3±17.</td>
<td>-18.6±3.1</td>
<td>4.84</td>
<td>$[81\text{BAR/CAC}]$</td>
</tr>
</tbody>
</table>
Parameters of the excess heat capacity. The units of the parameters are J K\(^{-1}\) kg\(^{-1}\) mol\(^{-1}\).

<table>
<thead>
<tr>
<th>Compound</th>
<th>(c_1)</th>
<th>(m_{\text{max}}/\text{mol kg}^{-1})</th>
<th>Workers</th>
</tr>
</thead>
<tbody>
<tr>
<td>sucrose</td>
<td>7.70±0.15</td>
<td>4.07</td>
<td>[76BON/CER]</td>
</tr>
</tbody>
</table>

Parameters of the excess volume. The units of the parameters are 10\(^{-6}\) m\(^3\) kg\(^{-1}\) mol\(^{-1}\).

<table>
<thead>
<tr>
<th>Compound</th>
<th>(v_1)</th>
<th>(v_2)</th>
<th>(m_{\text{max}}/\text{mol kg}^{-1})</th>
<th>Workers</th>
</tr>
</thead>
<tbody>
<tr>
<td>sucrose</td>
<td>0.534±0.03</td>
<td>2.08</td>
<td>[86BER/HOO]</td>
<td></td>
</tr>
<tr>
<td>sucrose</td>
<td>0.511±0.03</td>
<td>1.99</td>
<td>[86BER/HOO]</td>
<td></td>
</tr>
<tr>
<td>sucrose</td>
<td>0.37±0.1</td>
<td>0.44</td>
<td>[85UED/UED]</td>
<td></td>
</tr>
<tr>
<td>sucrose</td>
<td>0.782±0.23</td>
<td>5.10±0.056</td>
<td>3.00</td>
<td>[89UED/UED]</td>
</tr>
</tbody>
</table>

Parameters of the excess expansivity. The units of the parameters are 10\(^{-5}\) m\(^3\) K\(^{-1}\) kg\(^{-1}\) mol\(^{-1}\).

<table>
<thead>
<tr>
<th>Compound</th>
<th>(e_1)</th>
<th>(m_{\text{max}}/\text{mol kg}^{-1})</th>
<th>Workers</th>
</tr>
</thead>
<tbody>
<tr>
<td>sucrose</td>
<td>-1.2±0.3</td>
<td>2.08</td>
<td>[86BER/HOO]</td>
</tr>
<tr>
<td>sucrose</td>
<td>-0.9±0.5</td>
<td>1.99</td>
<td>[86BER/HOO]</td>
</tr>
</tbody>
</table>

Parameters of the excess isentropic compressibility. The units of the parameters are 10\(^{-15}\) m\(^3\) Pa\(^{-1}\) kg\(^{-1}\) mol\(^{-1}\).

<table>
<thead>
<tr>
<th>Compound</th>
<th>(k_{\text{st}})</th>
<th>(m_{\text{max}}/\text{mol kg}^{-1})</th>
<th>Workers</th>
</tr>
</thead>
<tbody>
<tr>
<td>sucrose</td>
<td>4.01±0.01</td>
<td>1.2</td>
<td>[86BER/HOO]</td>
</tr>
<tr>
<td>sucrose</td>
<td>2.73±0.01</td>
<td>0.4</td>
<td>[86BER/HOO]</td>
</tr>
</tbody>
</table>

Parameters of the temperature derivative of the excess isentropic compressibility. The units of the parameters are 10\(^{-15}\) m\(^3\) Pa\(^{-1}\) K\(^{-1}\) kg\(^{-1}\) mol\(^{-1}\).

<table>
<thead>
<tr>
<th>Compound</th>
<th>((k_{\text{st}}/\delta T)_h)</th>
<th>(m_{\text{max}}/\text{mol kg}^{-1})</th>
<th>Workers</th>
</tr>
</thead>
<tbody>
<tr>
<td>sucrose</td>
<td>-0.165±0.02</td>
<td>1.2</td>
<td>[86BER/HOO]</td>
</tr>
<tr>
<td>sucrose</td>
<td>-0.081±0.02</td>
<td>0.4</td>
<td>[86BER/HOO]</td>
</tr>
</tbody>
</table>

TABLE 7. Diffusion and viscosity data for aqueous carbohydrate solutions

Limiting values of the diffusion coefficients

<table>
<thead>
<tr>
<th>Carbohydrate</th>
<th>$T$/K</th>
<th>$D \times 10^{9}$/m$^2$/s</th>
<th>Workers</th>
</tr>
</thead>
<tbody>
<tr>
<td>fructose</td>
<td>298.15</td>
<td>7.001±0.01</td>
<td>[70UED/UEO]</td>
</tr>
<tr>
<td>glucose</td>
<td>298.15</td>
<td>6.735±0.05</td>
<td>[53GLA/DOL]; also see [55LON;</td>
</tr>
<tr>
<td></td>
<td>308.15</td>
<td>8.401±0.05</td>
<td>[53GLA/DOL]</td>
</tr>
<tr>
<td>ribose</td>
<td>298.15</td>
<td>7.795±0.01</td>
<td>[85UED/UEO]</td>
</tr>
<tr>
<td>xyllose</td>
<td>298.15</td>
<td>7.480±0.02</td>
<td>[69UED/UEO]</td>
</tr>
</tbody>
</table>

Expressions for the diffusion coefficients of aqueous carbohydrates as a function of concentration

<table>
<thead>
<tr>
<th>Carbohydrate</th>
<th>$T$/K</th>
<th>Expression ($D$ has units of $10^{9}$/m$^2$/s)</th>
<th>$m_{max}$/mol kg$^{-1}$ or $c_{max}$/mol L$^{-1}$</th>
<th>Workers</th>
</tr>
</thead>
<tbody>
<tr>
<td>fructose</td>
<td>298.15</td>
<td>$D = 7.00149 - 1.42416m$</td>
<td>0.14</td>
<td>[70UED/UEO]</td>
</tr>
<tr>
<td>glucose</td>
<td>298.15</td>
<td>$D = 67.3865 - 16.8107m + 2.60593m^2 - 0.250149m^3 + 0.0122802m^4 - 0.000226402m^5$</td>
<td>22.43</td>
<td>[53GLA/DOL]</td>
</tr>
<tr>
<td>ribose</td>
<td>308.15</td>
<td>$D = 84.0021 - 13.99043m + 0.87991m^2 - 0.0193112m^3$</td>
<td>25.08</td>
<td>[23GLA/UEO]</td>
</tr>
<tr>
<td>xyllose</td>
<td>298.15</td>
<td>$D = 7.79508 - 0.553466c$</td>
<td>0.16</td>
<td>[85UED/UEO]</td>
</tr>
</tbody>
</table>

Expressions for the reduced viscosities of aqueous carbohydrate solutions

<table>
<thead>
<tr>
<th>Carbohydrate</th>
<th>$T$/K</th>
<th>Expression</th>
<th>$c_{max}$/mol L$^{-1}$</th>
<th>Workers</th>
</tr>
</thead>
<tbody>
<tr>
<td>glucose</td>
<td>288.15</td>
<td>$(\eta/\eta^*) = 1.0 + 0.49c$</td>
<td>0.12</td>
<td>[83MTY/SAW;</td>
</tr>
<tr>
<td></td>
<td>298.15</td>
<td>$(\eta/\eta^*) = 1.0 + 0.45c$</td>
<td>0.17</td>
<td>[83MTY/SAW;</td>
</tr>
<tr>
<td></td>
<td>308.15</td>
<td>$(\eta/\eta^*) = 1.0 + 0.43c$</td>
<td>0.12</td>
<td>[83MTY/SAW;</td>
</tr>
<tr>
<td>xyllose</td>
<td>298.15</td>
<td>$(\eta/\eta^*) = (1.0 - 0.337c)^{-1}$</td>
<td>0.5</td>
<td>[69UED/UEO]</td>
</tr>
</tbody>
</table>

TABLE 8. Percent compositions of the anomeric forms of the hexoses and pentoses in D$_2$O. The data are taken from the review of [84ANG]

### A. Aldo-hexoses and pentoses

<table>
<thead>
<tr>
<th>Compound</th>
<th>$T$/K</th>
<th>pyranose $\alpha$</th>
<th>pyranose $\beta$</th>
<th>furanose $\alpha$</th>
<th>furanose $\beta$</th>
<th>aldehyde $eta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>arabinose</td>
<td>304.15</td>
<td>60.</td>
<td>35.5</td>
<td>2.5</td>
<td>2.</td>
<td>0.03</td>
</tr>
<tr>
<td>xylose</td>
<td>304.15</td>
<td>70.</td>
<td>28.</td>
<td>1.5</td>
<td>0.5</td>
<td>0.03</td>
</tr>
<tr>
<td>ribose</td>
<td>304.15</td>
<td>21.5</td>
<td>58.5</td>
<td>6.5</td>
<td>13.5</td>
<td>0.05</td>
</tr>
<tr>
<td>dulcose</td>
<td>304.15</td>
<td>36.5</td>
<td>63.</td>
<td>&lt;1</td>
<td></td>
<td>0.02</td>
</tr>
<tr>
<td>allose</td>
<td>304.15</td>
<td>14.</td>
<td>77.5</td>
<td>3.5</td>
<td>5.</td>
<td>0.01</td>
</tr>
<tr>
<td>altrose</td>
<td>295.15</td>
<td>27.</td>
<td>43.</td>
<td>17.</td>
<td>13.</td>
<td>0.04</td>
</tr>
<tr>
<td>galactose</td>
<td>304.15</td>
<td>30.</td>
<td>64.</td>
<td>2.5</td>
<td>3.5</td>
<td>0.02</td>
</tr>
<tr>
<td>glucose</td>
<td>304.15</td>
<td>38.</td>
<td>62.</td>
<td>—</td>
<td>0.14</td>
<td>0.002</td>
</tr>
<tr>
<td>gallose</td>
<td>295.15</td>
<td>16.</td>
<td>81.</td>
<td>—</td>
<td>3.</td>
<td>—</td>
</tr>
<tr>
<td>idose</td>
<td>304.15</td>
<td>38.5</td>
<td>36.</td>
<td>11.5</td>
<td>14.</td>
<td>0.2</td>
</tr>
<tr>
<td>mannose</td>
<td>317.15</td>
<td>65.5</td>
<td>34.5</td>
<td>0.6</td>
<td>0.3</td>
<td>0.005</td>
</tr>
<tr>
<td>talose</td>
<td>295.15</td>
<td>42.</td>
<td>29.</td>
<td>16.</td>
<td>13.</td>
<td>0.03</td>
</tr>
</tbody>
</table>

### B. Keto-hexoses

<table>
<thead>
<tr>
<th>Compound</th>
<th>$T$/K</th>
<th>pyranose $\alpha$</th>
<th>pyranose $\beta$</th>
<th>furanose $\alpha$</th>
<th>furanose $\beta$</th>
<th>keto form $\beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>fructose</td>
<td>303.15</td>
<td>2.</td>
<td>70.</td>
<td>5.</td>
<td>23.</td>
<td>0.7</td>
</tr>
<tr>
<td>psicose</td>
<td>300.15</td>
<td>22.</td>
<td>24.</td>
<td>39.</td>
<td>15.</td>
<td>0.2</td>
</tr>
<tr>
<td>sorbose</td>
<td>300.15</td>
<td>28.</td>
<td>2.</td>
<td>—</td>
<td>2.</td>
<td>0.2</td>
</tr>
<tr>
<td>tagatose</td>
<td>300.15</td>
<td>79.</td>
<td>16.</td>
<td>1.</td>
<td>4.</td>
<td>0.6</td>
</tr>
</tbody>
</table>

Table 9. Gibbs energy changes at 298.15 K for the conversion of the various forms of the carbohydrates to the equilibrium mixture. The units are kJ mol$^{-1}$.

<table>
<thead>
<tr>
<th>Carbohydrate</th>
<th>$\alpha$-pyranose</th>
<th>$\beta$-pyranose</th>
<th>$\alpha$-furanose</th>
<th>$\beta$-furanose</th>
<th>Enthalpy</th>
</tr>
</thead>
<tbody>
<tr>
<td>arabinose</td>
<td>+0.84</td>
<td>-0.44</td>
<td>-7.34</td>
<td>-7.87</td>
<td>-18</td>
</tr>
<tr>
<td>fucose</td>
<td>+0.83</td>
<td>-1.40</td>
<td>-6.58</td>
<td>-11.7</td>
<td>-19</td>
</tr>
<tr>
<td>ribose$^a$</td>
<td>-1.05</td>
<td>+1.45</td>
<td>-4.32</td>
<td>-2.48</td>
<td>-16</td>
</tr>
<tr>
<td>xylose</td>
<td>-0.77</td>
<td>+0.63</td>
<td>-5.86</td>
<td>-6.46</td>
<td>-20</td>
</tr>
<tr>
<td>allose</td>
<td>-3.03</td>
<td>+1.23</td>
<td>-6.78</td>
<td>-1.77</td>
<td>-16</td>
</tr>
<tr>
<td>altrose</td>
<td>-1.04</td>
<td>+1.04</td>
<td>-2.45</td>
<td>-1.94</td>
<td>-15</td>
</tr>
<tr>
<td>galactose</td>
<td>-0.86</td>
<td>+1.05</td>
<td>-5.58</td>
<td>-1.78</td>
<td>-16</td>
</tr>
<tr>
<td>glucose$^a$</td>
<td>-0.74</td>
<td>+0.49</td>
<td>-14.9</td>
<td>-20</td>
<td></td>
</tr>
<tr>
<td>galactose$^a$</td>
<td>3.12</td>
<td>+0.89</td>
<td>-7.1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>idose</td>
<td>+0.85</td>
<td>+0.70</td>
<td>-2.45</td>
<td>-1.94</td>
<td>-12</td>
</tr>
<tr>
<td>mannose</td>
<td>+0.71</td>
<td>-0.99</td>
<td>-11.8</td>
<td>-13.7</td>
<td>-24</td>
</tr>
<tr>
<td>talose</td>
<td>+0.99</td>
<td>+0.06</td>
<td>-1.25</td>
<td>-1.77</td>
<td>-17</td>
</tr>
</tbody>
</table>

$^a$In calculating these Gibbs energy changes it was necessary to estimate the percent compositions of a few isomers. These estimates were: 0.5% $\alpha$- and 0.5% $\beta$-furans of xylene; 0.1% $\alpha$- and 0.1% $\beta$-furans of glucose; 0.01% $\alpha$- and 0.005% $\beta$-furans of xylene; and 0.01% for the $\beta$-furanose form of sorbose. Where necessary estimated enthalpies were used to adjust the data in Table 8 to 298.15 K.

Table 10. Additional thermodynamic data for anemic conversions at 298.15 K

<table>
<thead>
<tr>
<th>Process</th>
<th>$\Delta G^\circ$</th>
<th>$\Delta H^\circ$</th>
<th>$\Delta S^\circ$</th>
<th>$\Delta V^\circ \times 10^{10}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>kJ mol$^{-1}$</td>
<td>J mol$^{-1}$ K$^{-1}$</td>
<td>m$^3$ mol$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>$\alpha$-xylose = $\alpha$-xylose</td>
<td>-1.40±0.2$^a$</td>
<td>-2.24±0.1$^a$</td>
<td>-2.8±0.8</td>
<td></td>
</tr>
<tr>
<td>$\alpha$-galactose = $\beta$-galactose</td>
<td>-1.90±0.2$^a$</td>
<td>-1.30±0.1$^c$</td>
<td>2.0±0.8</td>
<td></td>
</tr>
<tr>
<td>$\alpha$-glucose = $\beta$-glucose</td>
<td>-1.24±0.1$^a$</td>
<td>-1.15±0.05$^a$</td>
<td>0.30±0.4</td>
<td>-9±3$^f$                   0.31±0.02$^a$</td>
</tr>
<tr>
<td>$\alpha$-mannose = $\beta$-mannose</td>
<td>1.70±0.2$^a$</td>
<td>1.85±0.1$^f$</td>
<td>0.50±0.8</td>
<td></td>
</tr>
<tr>
<td>$\beta$-fructopyranose = $\beta$-fructofuranose</td>
<td>3.01±0.2$^a$</td>
<td>15.2±0.5$^f$</td>
<td>41.±2</td>
<td></td>
</tr>
</tbody>
</table>

$^a$Calculated from data in Table 8; adjustments to 298.15 K were done using the enthalpies given in this table.
$^b$Based on data given in [50KAD/PAT].
$^c$Based on data given in [73TAJ/ONO].
$^d$Based on data given in [41STU] and [58KAB/PAT].
$^e$Based on data given in [88BAL/SOM]; also see [65AND/GRO] and [66GRO/AND].
$^f$Based on data given in [41STU].
$^g$Based on data given in [66BER/HOO]; also see [25RIB].
<table>
<thead>
<tr>
<th>No.</th>
<th>Reaction</th>
<th>Property</th>
<th>Observed $\Delta H$ (kJ mol$^{-1}$)</th>
<th>Unc. $\Delta H$ (kJ mol$^{-1}$)</th>
<th>Residual $\Delta H$ (kJ mol$^{-1}$)</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6^{2-}$ (aq) + $\text{H}_2\text{O}$ (l) = $\text{C}<em>6\text{H}</em>{12}\text{O}_6^{2-}$ (aq) + $\text{HPO}_4^{2-}$ (aq)</td>
<td>$\Delta H$</td>
<td>0.91</td>
<td>0.35</td>
<td>-0.162</td>
<td>88TEW/ST3</td>
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<td>Calorimetric measurement using alkaline phosphatase</td>
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<td></td>
<td>Enthalpy of hydrolysis of glucose-6P</td>
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<td>2</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6^{2-}$ (aq) + $\text{H}_2\text{O}$ (l) = $\text{C}<em>6\text{H}</em>{12}\text{O}_6^{2-}$ (aq) + $\text{HPO}_4^{2-}$ (aq)</td>
<td>$\Delta G$</td>
<td>-1.63</td>
<td>0.7</td>
<td>0.571</td>
<td>49MEY/GRE</td>
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<td>Equilibrium constant for the hydrolysis of glucose-6P</td>
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<td></td>
<td>Adj. to 298.15 K using $\Delta H = 0.9$ kJ mol$^{-1}$ and</td>
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<td></td>
<td>$\Delta C_p = -48$ J mol$^{-1}$ K$^{-1}$; adj. from pH 7</td>
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<td>3</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6^{2-}$ (aq) + $\text{H}_2\text{O}$ (l) = $\text{C}<em>6\text{H}</em>{12}\text{O}_6^{2-}$ (aq) + $\text{HPO}_4^{2-}$ (aq)</td>
<td>$\Delta G$</td>
<td>-9.34</td>
<td>0.5</td>
<td>1031</td>
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<td>Equilibrium constant for the hydrolysis of glucose-6P</td>
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<td>Adj. from pH 7</td>
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<td>4</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6^{2-}$ (aq) + $\text{H}_2\text{O}$ (l) = $\text{C}<em>6\text{H}</em>{12}\text{O}_6^{2-}$ (aq) + $\text{HPO}_4^{2-}$ (aq)</td>
<td>$\Delta G$</td>
<td>-1.0</td>
<td>0.5</td>
<td>-2.129</td>
<td>61ATK/JOI</td>
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<td>Equilibrium constant for the hydrolysis of glucose-6P</td>
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<td>Adj. from pH 7</td>
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<td>5</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6^{2-}$ (aq) + $\text{H}_2\text{O}$ (l) = $\text{C}<em>6\text{H}</em>{12}\text{O}_6^{2-}$ (aq) + $\text{HPO}_4^{2-}$ (aq)</td>
<td>$\Delta G$</td>
<td>-14.80</td>
<td>0.10</td>
<td>0.071</td>
<td>79LAW/VIE</td>
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<td>Adj. to 298.15 K using $\Delta H = 0.9$ kJ mol$^{-1}$ and</td>
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<td>$\Delta C_p = -48$ J mol$^{-1}$ K$^{-1}$; adj. from pH 7</td>
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<td>6</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6^{2-}$ (aq3) + $\text{H}_2\text{O}$ (l) = $\text{C}<em>6\text{H}</em>{12}\text{O}_6^{2-}$ (aq2) + $\text{HPO}_4^{2-}$ (aq)</td>
<td>$\Delta H$</td>
<td>-1.4</td>
<td>0.3</td>
<td>0.000</td>
<td>88TEW/SIE</td>
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<td>Enthalpy of hydrolysis of mannose-6P</td>
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<td>7</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6^{2-}$ (aq3) + $\text{H}_2\text{O}$ (l) = $\text{C}<em>6\text{H}</em>{12}\text{O}_6^{2-}$ (aq2) + $\text{HPO}_4^{2-}$ (aq)</td>
<td>$\Delta G$</td>
<td>-9.08</td>
<td>0.70</td>
<td>0.000</td>
<td>49MEY/GRE</td>
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<td>Equilibrium constant for the hydrolysis of mannose-6P</td>
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<td>8</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6^{2-}$ (aq4) + $\text{H}_2\text{O}$ (l) = $\text{C}<em>6\text{H}</em>{12}\text{O}_6^{2-}$ (aq3) + $\text{HPO}_4^{2-}$ (aq)</td>
<td>$\Delta H$</td>
<td>-7.61</td>
<td>0.70</td>
<td>0.175</td>
<td>88TEW/SIE</td>
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<td>Enthalpy of hydrolysis of fructose-6P</td>
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<td>9</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6^{2-}$ (aq4) + $\text{H}_2\text{O}$ (l) = $\text{C}<em>6\text{H}</em>{12}\text{O}_6^{2-}$ (aq3) + $\text{HPO}_4^{2-}$ (aq)</td>
<td>$\Delta G$</td>
<td>-11.3</td>
<td>0.5</td>
<td>1.327</td>
<td>49MEY/GRE</td>
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<td>Equilibrium constant for the hydrolysis of fructose-6P</td>
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<td>Adj. from 38 °C using $\Delta H = -7.6$ kJ mol$^{-1}$, $\Delta C_p = -28$ J mol$^{-1}$ K$^{-1}$</td>
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<td>No.</td>
<td>Reaction</td>
<td>Property</td>
<td>Observed kJ mol(^{-1}) or J mol(^{-1}) K(^{-1})</td>
<td>Unc.</td>
<td>Residual</td>
<td>Reference</td>
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<td>10</td>
<td>(C_6H_12O_6^{2-}(aq4) + H_2O(l) = C_6H_12O_6(aq3) + HPO_4^{2-}(aq))</td>
<td>(\Delta G)</td>
<td>-13.70</td>
<td>0.30</td>
<td>-0.073</td>
<td>88TEW/STE</td>
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<td>Equilibrium measurement using alkaline phosphatase</td>
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<td>Equilibrium constant for the hydrolysis of fructose-6P</td>
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<td>11</td>
<td>(C_6H_12O_6P_2^{2-}(aq) + H_2O(l) = C_6H_12O_6(aq) + HPO_4^{2-}(aq))</td>
<td>(\Delta H)</td>
<td>-5.69</td>
<td>0.50</td>
<td>0.000</td>
<td>88TEW/STE</td>
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<td>Enthalpy of hydrolysis of ribose-5P</td>
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<td>12</td>
<td>(C_6H_12O_6P_2^{2-}(aq2) + H_2O(l) = C_6H_12O_6(aq2) + HPO_4^{2-}(aq))</td>
<td>(\Delta H)</td>
<td>-12.43</td>
<td>0.50</td>
<td>0.000</td>
<td>88TEW/STE</td>
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<td>Calorimetric measurement using alkaline phosphatase</td>
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<td>Enthalpy of hydrolysis of ribose-5P</td>
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<td>13</td>
<td>(C_6H_12O_6P_2^{2-}(aq5) + H_2O(l) = C_6H_12O_6(aq4) + HPO_4^{2-}(aq))</td>
<td>(\Delta G)</td>
<td>-11.15</td>
<td>0.70</td>
<td>0.000</td>
<td>49MEY/GRE</td>
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<td>Equilibrium constant for the hydrolysis of galactose-6P</td>
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<td>Adj. from 38 °C using (\Delta H = 1.5) kJ mol(^{-1}) and (\Delta C_p = -40) J mol(^{-1}) K(^{-1})</td>
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<td>14</td>
<td>(C_6H_12O_6P_2^{2-}(aq7) + H_2O(l) = C_6H_12O_6(aq3) + HPO_4^{2-}(aq))</td>
<td>(\Delta G)</td>
<td>-13.23</td>
<td>0.70</td>
<td>0.000</td>
<td>49MEY/GRE</td>
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<td>Equilibrium constant for the hydrolysis of fructose-1P</td>
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<td>Adj. from 38 °C using (\Delta H = -7.6) kJ mol(^{-1}) and (\Delta C_p = -28) J mol(^{-1}) K(^{-1})</td>
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<td>15</td>
<td>(C_6H_12O_6P_2^{2-}(aq5) + H_2O(l) = C_6H_12O_6(aq) + HPO_4^{2-}(aq))</td>
<td>(\Delta G)</td>
<td>-22.0</td>
<td>0.5</td>
<td>0.000</td>
<td>80CAM/GIR</td>
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<td>From cycle calc (two steps)</td>
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<td>Equil. constant for the hydrolysis of ribose-1P</td>
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<td>16</td>
<td>(C_6H_12O_6P_2^{2-}(aq) = C_6H_12O_6P_2^{2-}(aq4))</td>
<td>(\Delta H)</td>
<td>9.5</td>
<td>0.8</td>
<td>-2.168</td>
<td>50KAH/LOW</td>
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<td>Enthalpy of isomerization of glucose-6P to fructose-6P</td>
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<td>Secod law treatment</td>
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<td>17</td>
<td>(C_6H_12O_6P_2^{2-}(aq) = C_6H_12O_6P_2^{2-}(aq4))</td>
<td>(\Delta H)</td>
<td>11.7</td>
<td>0.2</td>
<td>0.032</td>
<td>88TEW/STE</td>
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<td>Calorimetric measurement using phosphoglucone isomerase</td>
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<td>Enthalpy of isomerization of glucose-6P to fructose-6P</td>
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<td>18</td>
<td>(C_6H_12O_6P_2^{2-}(aq) = C_6H_12O_6P_2^{2-}(aq4))</td>
<td>(\Delta G)</td>
<td>2.21</td>
<td>0.20</td>
<td>-0.937</td>
<td>50SLE</td>
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<td>Equil. constant for the isomerization of glucose-6P to fructose-6P</td>
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<td>Adj. from 30 °C using (\Delta H = 11.7) kJ mol(^{-1}) and (\Delta C_p = 44) J mol(^{-1}) K(^{-1})</td>
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<td>19</td>
<td>(C_6H_12O_6P_2^{2-}(aq) = C_6H_12O_6P_2^{2-}(aq4))</td>
<td>(\Delta G)</td>
<td>1.48</td>
<td>0.20</td>
<td>-0.667</td>
<td>56RAM/IR</td>
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<td>Equil. constant for the isomerization of glucose-6P to fructose-6P</td>
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<td>Adj. from 40 °C using (\Delta H = 11.7) kJ mol(^{-1}) and (\Delta C_p = 44) J mol(^{-1}) K(^{-1})</td>
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<td>26</td>
<td>C₆H₁₂O₆P²⁻ (ao) = C₆H₁₀O₇P²⁻ (ao4)</td>
<td>ΔG</td>
<td>1.44</td>
<td>0.20</td>
<td>-1.707</td>
<td>58NOL/BRU</td>
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<td>Equil. constant for the isomerization of glucose-6P to fructose-6P</td>
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<td>Adj. from 37 °C using ΔH = 11.7 kJ mol⁻¹ and ΔC_p = 44 J mol⁻¹ K⁻¹</td>
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<td>2</td>
<td>C₆H₁₂O₆P²⁻ (ao) = C₆H₁₀O₇P²⁻ (ao4)</td>
<td>ΔG</td>
<td>3.17</td>
<td>0.05</td>
<td>0.023</td>
<td>60KAH/LCW</td>
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<td>Equil. constant for the isomerization of glucose-6P to fructose-6P</td>
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<td>2i</td>
<td>C₆H₁₂O₆P²⁻ (ao3) = C₆H₁₀O₇P²⁻ (ao4)</td>
<td>ΔH</td>
<td>8.46</td>
<td>0.20</td>
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<td>68TEW/STE</td>
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<td>Equilibrium measurement using calorimetric data</td>
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<td>Equil. constant for the isomerization of glucose-6P to fructose-6P</td>
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<td>Calorimetric measurement using phosphomannose isomerase</td>
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<td>Enthalpy of isomerization of mannose-6P to fructose-6P</td>
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<td>2i</td>
<td>C₆H₁₂O₆P²⁻ (ao3) = C₆H₁₀O₇P²⁻ (ao4)</td>
<td>ΔG</td>
<td>-0.35</td>
<td>0.20</td>
<td>-0.875</td>
<td>50SLE</td>
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<td>Equil. constant for the isomerization of mannose-6P to fructose-6P</td>
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<td>Adj. from 30 °C using ΔH = 8.4 kJ mol⁻¹ and ΔC_p = 38 J mol⁻¹ K⁻¹</td>
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<td>2i</td>
<td>C₆H₁₂O₆P²⁻ (ao3) = C₆H₁₀O₇P²⁻ (ao4)</td>
<td>ΔG</td>
<td>-1.18</td>
<td>0.30</td>
<td>-1.205</td>
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<td>Equil. constant for the isomerization of mannose-6P to fructose-6P</td>
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<td>Adj. from 37 °C using ΔH = 8.4 kJ mol⁻¹ and ΔC_p = 38 J mol⁻¹ K⁻¹</td>
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<td>2i</td>
<td>C₆H₁₂O₆P²⁻ (ao3) = C₆H₁₀O₇P²⁻ (ao4)</td>
<td>ΔG</td>
<td>0.025</td>
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<td>Equil. constant for the isomerization of mannose-6P to fructose-6P</td>
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<td>C₆H₁₂O₆P²⁻ (ao2) = C₆H₁₀O₇P²⁻ (ao)</td>
<td>ΔH</td>
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<td>4.529</td>
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<td>Enthalpy of isomerization of ribulose-5P to ribose-5P</td>
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<td>ΔH</td>
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<td>4.529</td>
<td>54AXE/ION</td>
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<td>Enthalpy of isomerization of ribulose-5P to ribose-5P</td>
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<td>No.</td>
<td>Reaction</td>
<td>Property</td>
<td>Observed $\Delta H$ (kJ mol$^{-1}$)</td>
<td>Unc. $\Delta H$ (kJ mol$^{-1}$ K$^{-1}$)</td>
<td>Residual $\Delta C_p$ (kJ mol$^{-1}$ K$^{-1}$)</td>
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<td>29</td>
<td>C$<em>{6}$H$</em>{12}$O$<em>{6}$P$<em>2$$^-$ (aq2) = C$</em>{6}$H$</em>{12}$O$_{6}$P$_2$$^-$ (aq)</td>
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<td>Calorimetric measurement using phosphoribose isomerase</td>
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<td>C$<em>{6}$H$</em>{12}$O$<em>{6}$P$<em>2$$^-$ (aq2) = C$</em>{6}$H$</em>{12}$O$_{6}$P$_2$$^-$ (aq)</td>
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<td>31</td>
<td>C$<em>{6}$H$</em>{12}$O$<em>{6}$P$<em>2$$^-$ (aq2) = C$</em>{6}$H$</em>{12}$O$_{6}$P$_2$$^-$ (aq)</td>
<td>$\Delta G$</td>
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<td>-0.490</td>
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<td>Adj. from 37 °C using $\Delta H = -16.1$ kJ mol$^{-1}$ and $\Delta C_p = -40$ J mol$^{-1}$ K$^{-1}$</td>
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<td>32</td>
<td>C$<em>{6}$H$</em>{12}$O$<em>{6}$P$<em>2$$^-$ (aq2) = C$</em>{6}$H$</em>{12}$O$_{6}$P$_2$$^-$ (aq)</td>
<td>$\Delta G$</td>
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<td>Equil. const. for the isomerization of ribulose-5P to ribose-5P</td>
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<td>Adj. from 37 °C using $\Delta H = -16.1$ kJ mol$^{-1}$ and $\Delta C_p = -40$ J mol$^{-1}$ K$^{-1}$</td>
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<td>C$<em>{6}$H$</em>{12}$O$<em>{6}$P$<em>2$$^-$ (aq2) = C$</em>{6}$H$</em>{12}$O$_{6}$P$_2$$^-$ (aq)</td>
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<td>C$<em>{6}$H$</em>{12}$O$<em>{6}$P$<em>2$$^-$ (aq2) = C$</em>{6}$H$</em>{12}$O$_{6}$P$_2$$^-$ (aq)</td>
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<td>Adj. from 37 °C using $\Delta H = -16.1$ kJ mol$^{-1}$ and $\Delta C_p = -40$ J mol$^{-1}$ K$^{-1}$</td>
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<td>C$<em>{6}$H$</em>{12}$O$<em>{6}$P$<em>2$$^-$ (aq2) = C$</em>{6}$H$</em>{12}$O$_{6}$P$_2$$^-$ (aq)</td>
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<td>36</td>
<td>C$<em>{6}$H$</em>{12}$O$<em>{6}$P$<em>2$$^-$ (aq2) = C$</em>{6}$H$</em>{12}$O$_{6}$P$_2$$^-$ (aq)</td>
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<td>Adj. from 37 °C using $\Delta H = -16.1$ kJ mol$^{-1}$ and $\Delta C_p = -40$ J mol$^{-1}$ K$^{-1}$</td>
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<td>C$<em>{6}$H$</em>{12}$O$<em>{6}$P$<em>2$$^-$ (aq2) = C$</em>{6}$H$</em>{12}$O$_{6}$P$_2$$^-$ (aq)</td>
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<td>Adj. from 38 °C using $\Delta H = -16.1$ kJ mol$^{-1}$ and $\Delta C_p = -40$ J mol$^{-1}$ K$^{-1}$</td>
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<td>No.</td>
<td>Reaction</td>
<td>Property</td>
<td>Observed $\Delta G$ (kJ mol$^{-1}$ or J mol$^{-1}$ K$^{-1}$)</td>
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<td>38</td>
<td>$\text{C}_6\text{H}_5\text{O}_7\text{P}^{2-}(\text{ao2}) = \text{C}_6\text{H}_5\text{O}_7\text{P}^{2-}(\text{ao3})$</td>
<td>$\Delta G$</td>
<td>-0.19</td>
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<td>1.020</td>
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<td>Adj. from 24 °C using $\Delta H = +10.7$ kJ mol$^{-1}$ and $\Delta C_p = 0$ J mol$^{-1}$ K$^{-1}$</td>
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<td>$\text{C}_6\text{H}_5\text{O}_7\text{P}^{2-}(\text{ao2}) = \text{C}_6\text{H}_5\text{O}_7\text{P}^{2-}(\text{ao3})$</td>
<td>$\Delta G$</td>
<td>-0.19</td>
<td>0.50</td>
<td>1.020</td>
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<td>Adj. from 37 °C using $\Delta H = +10.7$ kJ mol$^{-1}$ and $\Delta C_p = 0$ J mol$^{-1}$ K$^{-1}$</td>
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<td>$\text{C}_6\text{H}_5\text{O}_7\text{P}^{2-}(\text{ao2}) = \text{C}_6\text{H}_5\text{O}_7\text{P}^{2-}(\text{ao3})$</td>
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<td>$\text{C}_6\text{H}_5\text{O}_7\text{P}^{2-}(\text{ao2}) = \text{C}_6\text{H}_5\text{O}_7\text{P}^{2-}(\text{ao3})$</td>
<td>$\Delta G$</td>
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<td>0.50</td>
<td>0.020</td>
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<td>Adj. from 37 °C using $\Delta H = +10.7$ kJ mol$^{-1}$ and $\Delta C_p = 0$ J mol$^{-1}$ K$^{-1}$</td>
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<td>42</td>
<td>$\text{C}_6\text{H}_5\text{O}_7\text{P}^{2-}(\text{ao2}) = \text{C}_6\text{H}_5\text{O}_7\text{P}^{2-}(\text{ao3})$</td>
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<td>Adj. from 37 °C using $\Delta H = +10.7$ kJ mol$^{-1}$ and $\Delta C_p = 0$ J mol$^{-1}$ K$^{-1}$</td>
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<td>$\text{C}_6\text{H}_5\text{O}_7\text{P}^{2-}(\text{ao2}) = \text{C}_6\text{H}_5\text{O}_7\text{P}^{2-}(\text{ao3})$</td>
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<td>Adj. from 24 °C using $\Delta H = +10.7$ kJ mol$^{-1}$ and $\Delta C_p = 0$ J mol$^{-1}$ K$^{-1}$</td>
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<td>$\text{C}_6\text{H}_5\text{O}_7\text{P}^{2-}(\text{ao2}) = \text{C}_6\text{H}_5\text{O}_7\text{P}^{2-}(\text{ao3})$</td>
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<td>$\text{C}_6\text{H}_5\text{O}_7\text{P}^{2-}(\text{ao2}) = \text{C}_6\text{H}_5\text{O}_7\text{P}^{2-}(\text{ao3})$</td>
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<td>Adj. from 35 °C using $\Delta H = +10.7$ kJ mol$^{-1}$ and $\Delta C_p = 0$ J mol$^{-1}$ K$^{-1}$</td>
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<td>$\text{C}_6\text{H}_5\text{O}_7\text{P}^{2-}(\text{ao4}) = \text{C}_6\text{H}_5\text{O}_7\text{P}^{2-}(\text{ao2})$</td>
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<td>0.000</td>
<td>66VOL</td>
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<td>Equil constant for the isomerization of arabinose-5P to ribulose-5P</td>
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<td>Adj. from 38 °C using $\Delta H = 25.0$ kJ mol$^{-1}$ and $\Delta C_p = 0$ J mol$^{-1}$ K$^{-1}$</td>
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<td>No.</td>
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<td>Property</td>
<td>Observed $\Delta G$</td>
<td>Unc. $</td>
<td>\Delta G</td>
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<td>47</td>
<td>C$<em>6$H$</em>{12}$O$_5$P$_2$-(ao2) = C$<em>6$H$</em>{11}$O$_5$P$_2$-(ao)</td>
<td>$\Delta G$</td>
<td>-7.13</td>
<td>0.20</td>
<td>-0.055</td>
<td>42COL/SUT</td>
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<td>Equil. constant for the isomerization o' glucose-1P to glucose-6P</td>
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<td>48</td>
<td>C$<em>6$H$</em>{12}$O$_5$P$_2$-(ao2) = C$<em>6$H$</em>{11}$O$_5$P$_2$-(ao)</td>
<td>$\Delta G$</td>
<td>-7.9</td>
<td>0.5</td>
<td>-0.825</td>
<td>61BEN/SCH</td>
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<td></td>
<td>Equil. measurement</td>
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<td>Equil. constant for the isomerization o' glucose-1P to glucose-6P</td>
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<td>Equil. measurement determined at 310.15 K. adjusted to</td>
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<td>298.15 K using $\Delta H = 0$ kJ mol$^{-1}$</td>
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<td>49</td>
<td>C$<em>6$H$</em>{12}$O$_5$P$_2$-(ao2) = C$<em>6$H$</em>{11}$O$_5$P$_2$-(ao)</td>
<td>$\Delta G$</td>
<td>-7.02</td>
<td>0.20</td>
<td>0.055</td>
<td>61ATK/JOH</td>
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<td>Equil. measurement</td>
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<td>Equil. constant for the isomerization o' glucose-1P to glucose-6P</td>
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<td>50</td>
<td>C$<em>6$H$</em>{12}$O$_5$P$_2$-(ao5) = C$<em>6$H$</em>{11}$O$_5$P$_2$-(ao2)</td>
<td>$\Delta G$</td>
<td>-2.8</td>
<td>0.5</td>
<td>0.000</td>
<td>52LEL/CAR</td>
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<td>Equil. constant for the isomerization o' galactose-1P to glucose-1P</td>
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<td>Equil. measurement at 37 °C. value uncorrected.</td>
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<td>51</td>
<td>C$<em>6$H$</em>{12}$O$_6$(ao) = C$<em>6$H$</em>{12}$O$_6$(ao3)</td>
<td>$\Delta H$</td>
<td>8.9</td>
<td>2.0</td>
<td>6.088</td>
<td>67TAK</td>
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<td>Enthalpy of isomerization of glucose to fructose</td>
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<td>52</td>
<td>C$<em>6$H$</em>{12}$O$_6$(ao) = C$<em>6$H$</em>{12}$O$_6$(ao3)</td>
<td>$\Delta H$</td>
<td>0.4</td>
<td>3.0</td>
<td>-2.412</td>
<td>73HAV/PIT</td>
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<td>Enthalpy of isomerization of glucose to fructose</td>
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<td>53</td>
<td>C$<em>6$H$</em>{12}$O$_6$(ao) = C$<em>6$H$</em>{12}$O$_6$(ao3)</td>
<td>$\Delta H$</td>
<td>6.0</td>
<td>2.0</td>
<td>3.188</td>
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<td>Enthalpy of isomerization of glucose to fructose</td>
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<td>54</td>
<td>C$<em>6$H$</em>{12}$O$_6$(ao) = C$<em>6$H$</em>{12}$O$_6$(ao3)</td>
<td>$\Delta H$</td>
<td>1.5</td>
<td>4.0</td>
<td>-1.312</td>
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<td>55</td>
<td>C$<em>6$H$</em>{12}$O$_6$(ao) = C$<em>6$H$</em>{12}$O$_6$(ao3)</td>
<td>$\Delta H$</td>
<td>3.1</td>
<td>2.0</td>
<td>0.288</td>
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<tr>
<td>No.</td>
<td>Reaction</td>
<td>Property</td>
<td>Observed $\Delta H$ (kJ mol$^{-1}$ or J mol$^{-1}$ K$^{-1}$)</td>
<td>Unc.</td>
<td>Residual</td>
<td>Reference</td>
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<td>56</td>
<td>$C_6H_{12}O_6(aq) = C_6H_{12}O_6(aq3)^{-}$</td>
<td>$\Delta H$</td>
<td>7.1</td>
<td>1.0</td>
<td>4.288</td>
<td>76SPR/LIM</td>
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<td>Enthalpy of isomerization of glucose to fructose</td>
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<td>57</td>
<td>$C_6H_{12}O_6(aq) = C_6H_{12}O_6(aq3)^{-}$</td>
<td>$\Delta H$</td>
<td>2.9</td>
<td>15.0</td>
<td>0.088</td>
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<td>Enthalpy of isomerization of glucose to fructose</td>
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<td>58</td>
<td>$C_6H_{12}O_6(aq) = C_6H_{12}O_6(aq3)^{-}$</td>
<td>$\Delta H$</td>
<td>6.3</td>
<td>20.0</td>
<td>3.488</td>
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<td>Enthalpy of isomerization of glucose to fructose</td>
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<td>59</td>
<td>$C_6H_{12}O_6(aq) = C_6H_{12}O_6(aq3)^{-}$</td>
<td>$\Delta H$</td>
<td>2.6</td>
<td>0.6</td>
<td>-0.212</td>
<td>83TIL</td>
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<td>Enthalpy of isomerization of glucose to fructose</td>
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<td>60</td>
<td>$C_6H_{12}O_6(aq) = C_6H_{12}O_6(aq3)^{-}$</td>
<td>$\Delta H$</td>
<td>2.7</td>
<td>0.7</td>
<td>-0.112</td>
<td>84LLO/CHA</td>
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<td>Enthalpy of isomerization of glucose to fructose</td>
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<td>61</td>
<td>$C_6H_{12}O_6(aq) = C_6H_{12}O_6(aq3)^{-}$</td>
<td>$\Delta H$</td>
<td>2.6</td>
<td>0.3</td>
<td>-0.212</td>
<td>84TEW/GOL</td>
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<td>Enthalpy of isomerization of glucose to fructose</td>
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<td>62</td>
<td>$C_6H_{12}O_6(aq) = C_6H_{12}O_6(aq3)^{-}$</td>
<td>$\Delta H$</td>
<td>2.78</td>
<td>0.20</td>
<td>-0.032</td>
<td>84TEW/GOL</td>
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<td>Enthalpy of isomerization of glucose to fructose</td>
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<tr>
<td>63</td>
<td>$C_6H_{12}O_6(aq) = C_6H_{12}O_6(aq3)^{-}$</td>
<td>$\Delta H$</td>
<td>3.7</td>
<td>0.8</td>
<td>0.888</td>
<td>86OLI/TOI</td>
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<td>Enthalpy of isomerization of glucose to fructose</td>
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<td></td>
<td>Adjusted to 298.15 K using $\Delta C_p = 76$ J mol$^{-1}$ K$^{-1}$</td>
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<tr>
<td>No.</td>
<td>Reaction</td>
<td>Property</td>
<td>Observed ( \Delta G )</td>
<td>Unc. ( kJ \text{ mol}^{-1} \text{ or } J \text{ mol}^{-1} \text{ K}^{-1} )</td>
<td>Residual</td>
<td>Reference</td>
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<td>64</td>
<td>( \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao3}) )</td>
<td>( \Delta G )</td>
<td>0.50</td>
<td>0.30</td>
<td>1.110</td>
<td>67DAN/YOS</td>
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<td>Equil constant for the isomerization of glucose to fructose</td>
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<td></td>
<td>Adjusted to 298 K using ( \Delta H = 2.78 ) kJ mol(^{-1}) and ( \Delta C_p = 76 ) J mol(^{-1}) K(^{-1})</td>
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<td>65</td>
<td>( \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao3}) )</td>
<td>( \Delta G )</td>
<td>0.71</td>
<td>0.20</td>
<td>0.320</td>
<td>67TAK</td>
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<td>66</td>
<td>( \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao3}) )</td>
<td>( \Delta G )</td>
<td>0.14</td>
<td>0.60</td>
<td>-0.250</td>
<td>73HAV/PIT</td>
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<td>Equil constant for the isomerization of glucose to fructose</td>
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<td>67</td>
<td>( \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao3}) )</td>
<td>( \Delta G )</td>
<td>0.55</td>
<td>3.00</td>
<td>0.160</td>
<td>74LAN</td>
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<td>68</td>
<td>( \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao3}) )</td>
<td>( \Delta G )</td>
<td>0.35</td>
<td>0.70</td>
<td>-0.070</td>
<td>74SCA/SHI</td>
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<td>Equil constant for the isomerization of glucose to fructose</td>
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<td>69</td>
<td>( \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao3}) )</td>
<td>( \Delta G )</td>
<td>0.41</td>
<td>0.20</td>
<td>0.020</td>
<td>76LLO/KHA</td>
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<td>Equil constant for the isomerization of glucose to fructose</td>
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<td>70</td>
<td>( \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao3}) )</td>
<td>( \Delta G )</td>
<td>0.58</td>
<td>0.10</td>
<td>0.190</td>
<td>76SPR/LIM</td>
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<td>71</td>
<td>( \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao3}) )</td>
<td>( \Delta G )</td>
<td>0.37</td>
<td>2.00</td>
<td>-0.020</td>
<td>79CLI</td>
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<td>Equil constant for the isomerization of glucose to fructose</td>
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<td>72</td>
<td>( \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao3}) )</td>
<td>( \Delta G )</td>
<td>0.97</td>
<td>3.00</td>
<td>0.580</td>
<td>79MCK/TAV</td>
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<tr>
<td>No.</td>
<td>Reaction</td>
<td>Property</td>
<td>Observed $\Delta G$ (kJ mol$^{-1}$)</td>
<td>Unc. $\Delta G$ (kJ mol$^{-1}$)</td>
<td>Residual $\Delta G$ (kJ mol$^{-1}$)</td>
<td>Reference</td>
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<td>3</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(aq) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(aq3)$</td>
<td>$\Delta G$</td>
<td>0.36</td>
<td>0.10</td>
<td>-0.090</td>
<td>13TIL</td>
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<td>Equil. constant for the isomerization of glucose to fructose</td>
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<td>4</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(aq) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(aq3)$</td>
<td>$\Delta G$</td>
<td>0.41</td>
<td>0.20</td>
<td>0.020</td>
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<td>5</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(aq) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(aq3)$</td>
<td>$\Delta G$</td>
<td>0.340</td>
<td>0.050</td>
<td>-0.041</td>
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<td>6</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(aq) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(aq3)$</td>
<td>$\Delta G$</td>
<td>0.44</td>
<td>0.08</td>
<td>0.050</td>
<td>16OLI/TOI</td>
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<td>Adjusted to 298.15 K using $\Delta G_f = 76 \text{ J mol}^{-1} \text{ K}^{-1}$</td>
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<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(aq2) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(aq3)$</td>
<td>$\Delta H$</td>
<td>0.0</td>
<td>2.0</td>
<td>0.725</td>
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<td>Enthalpy of isomerization of mannose to fructose</td>
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<td>8</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(aq2) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(aq3)$</td>
<td>$\Delta G$</td>
<td>-2.12</td>
<td>0.50</td>
<td>2.302</td>
<td>56PAL/DOU</td>
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<td>Adj. from 30 °C using $\Delta H = 0.0 \text{ kJ mol}^{-1}$</td>
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<td>7</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(aq2) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(aq3)$</td>
<td>$\Delta G$</td>
<td>-2.72</td>
<td>0.20</td>
<td>1.802</td>
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<td>8</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(aq) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(aq5)$</td>
<td>$\Delta H$</td>
<td>-9.3</td>
<td>3.0</td>
<td>-0.017</td>
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<td>Enthalpy of isomerization of ribose to arabinose</td>
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<td>8</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(aq) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(aq5)$</td>
<td>$\Delta G$</td>
<td>-3.44</td>
<td>0.30</td>
<td>0.000</td>
<td>85TEW/GCL</td>
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<td>Equil. constant for the isomerization of ribose to arabinose</td>
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<td>No.</td>
<td>Reaction</td>
<td>Property</td>
<td>Observed $\Delta H$ (kJ mol$^{-1}$)</td>
<td>Unc. $\Delta H$ (kJ mol$^{-1}$)</td>
<td>Residual</td>
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<tr>
<td>82</td>
<td>$C_6H_12O_5(aq) = C_6H_12O_6(aq)$</td>
<td>$\Delta H$</td>
<td>11.0</td>
<td>2.0</td>
<td>0.011</td>
<td>85TEW/GOL</td>
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<td>Enthalpy of isomerization of ribose to ribulose</td>
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<tr>
<td>83</td>
<td>$C_6H_12O_6(aq) = C_6H_12O_6(aq)$</td>
<td>$\Delta G$</td>
<td>2.85</td>
<td>0.20</td>
<td>0.000</td>
<td>85TEW/GOL</td>
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<td>Equil. constant for the isomerization of ribose to ribulose</td>
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<td>84</td>
<td>$C_6H_12O_6(aq)$</td>
<td>$\Delta H$</td>
<td>22.3</td>
<td>4.0</td>
<td>6.210</td>
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<td>Enthalpy for the isomerization of xylene to xylolose</td>
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<td>85</td>
<td>$C_6H_12O_6(aq)$</td>
<td>$\Delta H$</td>
<td>16.09</td>
<td>0.70</td>
<td>0.000</td>
<td>85TEW/STE</td>
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<td>Enthalpy of isomerization of xylose to xylolose</td>
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<td>86</td>
<td>$C_6H_12O_6(aq)$</td>
<td>$\Delta H$</td>
<td>18.8</td>
<td>6.0</td>
<td>2.710</td>
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<td>Enthalpy of isomerization of xylose to xylolose</td>
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<td>87</td>
<td>$C_6H_12O_6(aq)$</td>
<td>$\Delta G$</td>
<td>4.22</td>
<td>0.50</td>
<td>-0.113</td>
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<td>Equil. constant for the isomerization of xylene to xylolose</td>
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<td>Adj. from 27 °C using $\Delta H = 16.09$ kJ mol$^{-1}$</td>
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<td>88</td>
<td>$C_6H_12O_6(aq)$</td>
<td>$\Delta G$</td>
<td>4.38</td>
<td>0.50</td>
<td>0.087</td>
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<td>Adj. from 30 °C using $\Delta H = 16.09$ kJ mol$^{-1}$</td>
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<td>89</td>
<td>$C_6H_12O_6(aq)$</td>
<td>$\Delta G$</td>
<td>5.37</td>
<td>0.50</td>
<td>1.087</td>
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<td>90</td>
<td>$C_6H_12O_6(aq)$</td>
<td>$\Delta G$</td>
<td>4.389</td>
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<td>0.086</td>
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<td>Reaction</td>
<td>Property</td>
<td>Observed $\Delta G$ (kJ mol$^{-1}$)</td>
<td>Unc. $\Delta G$ (kJ mol$^{-1}$)</td>
<td>Residual $\Delta G$ (kJ mol$^{-1}$)</td>
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<td>91</td>
<td>$\text{C}<em>6\text{H}</em>{10}\text{O}_5$(a03) = $\text{C}<em>6\text{H}</em>{10}\text{O}_5$(a04)</td>
<td>$\Delta G$</td>
<td>4.99</td>
<td>0.55</td>
<td>0.657</td>
<td>86OLI/TOI</td>
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<td>Equil. constant for the isomerization of xyllose to xylose</td>
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<td>Adjusted to 298.15 K using $\Delta G^\circ = 40 \text{ J mol}^{-1} \text{ K}^{-1}$</td>
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<td>92</td>
<td>$\text{C}<em>6\text{H}</em>{10}\text{O}_5$(a05) = $\text{C}<em>6\text{H}</em>{10}\text{O}_5$(a02)</td>
<td>$\Delta H$</td>
<td>20.75</td>
<td>4.00</td>
<td>-3.022</td>
<td>86TEW/GOL</td>
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<td></td>
<td>Enthalpy of isomerization of arabinose to ribulose</td>
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<td>93</td>
<td>$\text{C}<em>6\text{H}</em>{10}\text{O}_5$(a05) = $\text{C}<em>6\text{H}</em>{10}\text{O}_5$(a02)</td>
<td>$\Delta G$</td>
<td>5.10</td>
<td>0.50</td>
<td>-1.190</td>
<td>55COH</td>
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<td>Equil. constant for the isomerization of aabinose to ribulose</td>
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<td>Adj. from 37 °C using $\Delta H = -20.75 \text{ kJ mol}^{-1}$</td>
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<td>94</td>
<td>$\text{C}<em>6\text{H}</em>{10}\text{O}_5$(a05) = $\text{C}<em>6\text{H}</em>{10}\text{O}_5$(a02)</td>
<td>$\Delta G$</td>
<td>6.29</td>
<td>0.40</td>
<td>0.000</td>
<td>85TEW/STE</td>
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<td>Equil. constant for the isomerization of aabinose to ribulose</td>
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<td>95</td>
<td>$\text{C}<em>6\text{H}</em>{10}\text{O}_5$(a06) = $\text{C}<em>6\text{H}</em>{10}\text{O}_5$(a07)</td>
<td>$\Delta H$</td>
<td>7.42</td>
<td>2.00</td>
<td>1.190</td>
<td>85TEW/STE</td>
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<td></td>
<td>Second law treatment</td>
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<td></td>
<td>Enthalpy of isomerization of allose to psicose</td>
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<td></td>
<td>No solution for variable or data missing</td>
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<td>95</td>
<td>$\text{C}<em>6\text{H}</em>{10}\text{O}_5$(a06) = $\text{C}<em>6\text{H}</em>{10}\text{O}_5$(a07)</td>
<td>$\Delta G$</td>
<td>-1.41</td>
<td>0.10</td>
<td>-0.000</td>
<td>85TEW/GOL</td>
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<td>Equilibrium measurement</td>
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<td>Equil. constant for the isomerization of allose to psicose</td>
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<td>97</td>
<td>$\text{C}<em>6\text{H}</em>{10}\text{O}_5$(a07) = $\text{C}<em>6\text{H}</em>{10}\text{O}_5$(a09)</td>
<td>$\Delta G$</td>
<td>3.4</td>
<td>0.1</td>
<td>0.000</td>
<td>85TEW/GOL</td>
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<td>Equil. constant for the isomerization of psicose to allose</td>
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<tr>
<td>98</td>
<td>$\text{C}<em>6\text{H}</em>{10}\text{O}_5$(a04) = $\text{C}<em>6\text{H}</em>{10}\text{O}_5$(a08)</td>
<td>$\Delta G$</td>
<td>-2.33</td>
<td>0.50</td>
<td>0.455</td>
<td>55PAL/DOU</td>
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<td>Equilibrium measurement</td>
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<td>Equil. constant for the isomerization of xyllose to lyxose</td>
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<td></td>
<td>Assume $K(298.15 \text{ K}) = K(30\text{.15 K})$</td>
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<tr>
<td>No.</td>
<td>Reaction</td>
<td>Property</td>
<td>Observed ( \Delta G ) or ( \Delta H )</td>
<td>Unc.</td>
<td>Residual</td>
<td>Reference</td>
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<td>99</td>
<td>( \text{C}_6\text{H}_12\text{O}_6(\text{aq}) = \text{C}_6\text{H}_12\text{O}_6(\text{aq}) )</td>
<td>( \Delta G )</td>
<td>-3.64</td>
<td>0.50</td>
<td>-0655</td>
<td>65AND/ALL</td>
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<td>Equilibrium measurement</td>
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<td>Equil. constant for the isomerization of xylose to lyxose</td>
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<td>100</td>
<td>( \text{C}_6\text{H}_12\text{N}_5\text{O}_7\text{P}^{3-}(\text{ao}) + \text{H}_2\text{O}(\text{l}) = \text{C}_6\text{H}_12\text{N}_5\text{O}_7\text{P}^{3-}(\text{ao}) )</td>
<td>( \Delta H )</td>
<td>-22.3</td>
<td>3.0</td>
<td>-1800</td>
<td>55KIT/BEN</td>
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<td></td>
<td>+ ( \text{HPO}^4^-\text{(ao)} + \text{H}^+(\text{ao}) )</td>
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<td>Calorimetric measurement</td>
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<td>Enthalpy of hydrolysis of ATP</td>
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<td></td>
<td>Adj. to 298.15 K with ( \Delta H = -21.5 \text{ kJ mol}^{-1} ) and</td>
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<td></td>
<td>( \Delta C_p = -237 \text{ J mol}^{-1} \text{ K}^{-1} ). Corr. to std.</td>
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<td>101</td>
<td>( \text{C}_6\text{H}_12\text{N}_5\text{O}_7\text{P}^{3-}(\text{ao}) + \text{H}_2\text{O}(\text{l}) = \text{C}_6\text{H}_12\text{N}_5\text{O}_7\text{P}^{3-}(\text{ao}) )</td>
<td>( \Delta H )</td>
<td>-22.3</td>
<td>3.0</td>
<td>-1800</td>
<td>5POD/MOR</td>
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<td>+ ( \text{HPO}^4^-\text{(ao)} + \text{H}^+(\text{ao}) )</td>
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<td>Adj. to 298.15 K with ( \Delta H = -21.5 \text{ kJ mol}^{-1} ) and</td>
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<td>( \Delta C_p = -237 \text{ J mol}^{-1} \text{ K}^{-1} ). Corr. to std.</td>
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<td>102</td>
<td>( \text{C}_6\text{H}_12\text{N}_5\text{O}_7\text{P}^{3-}(\text{ao}) + \text{H}_2\text{O}(\text{l}) = \text{C}_6\text{H}_12\text{N}_5\text{O}_7\text{P}^{3-}(\text{ao}) )</td>
<td>( \Delta H )</td>
<td>-19.0</td>
<td>3.0</td>
<td>1.500</td>
<td>55POD/STU</td>
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<td>+ ( \text{HPO}^4^-\text{(ao)} + \text{H}^+(\text{ao}) )</td>
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<td>Calorimetric measurement</td>
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<td>Enthalpy of hydrolysis of ATP</td>
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<td>Adj. to 298.15 K with ( \Delta H = -21.5 \text{ kJ mol}^{-1} ) and</td>
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<td>( \Delta C_p = -237 \text{ J mol}^{-1} \text{ K}^{-1} ). Corr. to std.</td>
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<td>state is uncertain</td>
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<td>103</td>
<td>( \text{C}_6\text{H}_12\text{N}_5\text{O}_7\text{P}^{3-}(\text{ao}) + \text{H}_2\text{O}(\text{l}) = \text{C}_6\text{H}_12\text{N}_5\text{O}_7\text{P}^{3-}(\text{ao}) )</td>
<td>( \Delta H )</td>
<td>-20.5</td>
<td>0.4</td>
<td>0.000</td>
<td>86GAI/STE</td>
</tr>
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<td></td>
<td>+ ( \text{HPO}^4^-\text{(ao)} + \text{H}^+(\text{ao}) )</td>
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<td>Calorimetric measurement</td>
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<td>Enthalpy of hydrolysis of ATP</td>
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<td>104</td>
<td>( \text{C}_6\text{H}_12\text{N}_5\text{O}_7\text{P}^{3-}(\text{ao}) + \text{H}_2\text{O}(\text{l}) = \text{C}_6\text{H}_12\text{N}_5\text{O}_7\text{P}^{3-}(\text{ao}) )</td>
<td>( \Delta G )</td>
<td>3.03</td>
<td>0.50</td>
<td>0.000</td>
<td>73GUY/VEE</td>
</tr>
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<td></td>
<td>+ ( \text{HPO}^4^-\text{(ao)} + \text{H}^+(\text{ao}) )</td>
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<td>Equilibrium Measurement</td>
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<td></td>
<td>Equil. constant for the hydrolysis of ATP</td>
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<td>105</td>
<td>( \text{C}_6\text{H}_12\text{O}(\text{ao}) + \text{C}_6\text{H}_12\text{N}_5\text{O}_7\text{P}^{3-}(\text{ao}) = \text{C}_6\text{H}_12\text{O}_6\text{P}^{3-}(\text{ao}) + \text{C}_9\text{H}_12\text{N}_5\text{O}_7\text{P}^{2-3}(\text{ao}) + \text{H}^+(\text{ao}) )</td>
<td>( \Delta H )</td>
<td>-23.8</td>
<td>0.7</td>
<td>-2228</td>
<td>75GOL</td>
</tr>
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<td></td>
<td>Calorimetric measurement</td>
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<td>Enthalpy of phosphorylation (ATP) of glucose</td>
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<tr>
<td>No.</td>
<td>Reaction</td>
<td>Property</td>
<td>Observed kJ mol(^{-1}) or J mol(^{-1}) K(^{-1})</td>
<td>Unc.</td>
<td>Residual</td>
<td>Reference</td>
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<td>106</td>
<td>(\text{C}_4\text{H}_7\text{O}_5\text{(so) + C}_6\text{H}_4\text{O}_2\text{P}^{3-}\text{(ao)} = C}_4\text{H}_7\text{O}_5\text{P}^{3-}\text{(ao) + C}_6\text{H}_4\text{O}_2\text{P}^{3-}\text{(ao) + H}^{+}\text{(ao)})</td>
<td>(\Delta H)</td>
<td>-234</td>
<td>2.0</td>
<td>-1.828</td>
<td>75MCG/JOR</td>
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<td>Enthalpy of phosphorylation (ATP) of glucose</td>
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<td>Calorimetric measurement</td>
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<td></td>
<td>Data adjusted using information on the magnesium dependency of the measured enthalpy see 76GOL</td>
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<td>107</td>
<td>(\text{C}_6\text{H}_12\text{O}_6\text{(so) + C}_6\text{H}_2\text{N}_2\text{O}_7\text{P}^{3-}\text{(ao)} = C}_6\text{H}_12\text{O}_6\text{P}^{3-}\text{(ao) + C}_6\text{H}_2\text{N}_2\text{O}_7\text{P}^{3-}\text{(ao) + H}^{+}\text{(ao)})</td>
<td>(\Delta G)</td>
<td>19.0</td>
<td>0.5</td>
<td>5.099</td>
<td>57ROB/BOY</td>
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<td>Equilibrium constant for the phosphorylation (ATP) of glucose</td>
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<td>108</td>
<td>(\text{C}_6\text{H}_12\text{O}_6\text{(so) + C}_6\text{H}_2\text{N}_2\text{O}_7\text{P}^{3-}\text{(ao)} = C}_6\text{H}_12\text{O}_6\text{P}^{3-}\text{(ao) + C}_6\text{H}_2\text{N}_2\text{O}_7\text{P}^{3-}\text{(ao) + H}^{+}\text{(ao)})</td>
<td>(\Delta G)</td>
<td>21.0</td>
<td>4.0</td>
<td>7.099</td>
<td>57VLA</td>
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<td>Equilibrium constant for the phosphorylation (ATP) of glucose</td>
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<td>Approx: (\Delta G) since metal conc. and ion. strength not given</td>
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<td>109</td>
<td>(\text{C}_6\text{H}_12\text{O}_6\text{(so2) + C}_6\text{H}_2\text{N}_2\text{O}_7\text{P}^{3-}\text{(ao)} = C}_6\text{H}_12\text{O}_6\text{P}^{3-}\text{(ao3) + C}_6\text{H}_2\text{N}_2\text{O}_7\text{P}^{3-}\text{(ao) + H}^{+}\text{(ao)})</td>
<td>(\Delta H)</td>
<td>-213</td>
<td>0.7</td>
<td>0.000</td>
<td>75GOL</td>
</tr>
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<td>Calorimetric measurement</td>
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<td>Enthalpy of phosphorylation (ATP) of fructose</td>
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<td>110</td>
<td>(\text{C}_6\text{H}_12\text{O}_6\text{(so3) + C}_6\text{H}_2\text{N}_2\text{O}_7\text{P}^{3-}\text{(ao)} = C}_6\text{H}_12\text{O}_6\text{P}^{3-}\text{(ao4) + C}_6\text{H}_2\text{N}_2\text{O}_7\text{P}^{3-}\text{(ao) + H}^{+}\text{(ao)})</td>
<td>(\Delta H)</td>
<td>-153</td>
<td>0.9</td>
<td>-2.285</td>
<td>75GOL</td>
</tr>
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<td>Enthalpy of phosphorylation (ATP) of fructose</td>
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<td>111</td>
<td>(\text{C}_6\text{H}_12\text{O}_6\text{(so4) + C}_6\text{H}_2\text{N}_2\text{O}_7\text{P}^{3-}\text{(ao)} = C}_6\text{H}_12\text{O}_6\text{P}^{3-}\text{(ao6) + C}_6\text{H}_2\text{N}_2\text{O}_7\text{P}^{3-}\text{(ao) + H}^{+}\text{(ao)})</td>
<td>(\Delta G)</td>
<td>25.8</td>
<td>2.0</td>
<td>8.893</td>
<td>61ATK/BUR</td>
</tr>
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<td>Equil. const. for the phosphorylation (ATP) of galactose to galactose-1P</td>
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<tr>
<td>112</td>
<td>(\text{C}_6\text{H}_12\text{O}_6\text{(cr3) 3rd law entropy of xylose(cr)})</td>
<td>S</td>
<td>143.5</td>
<td>10.0</td>
<td>0.000</td>
<td>31MIL</td>
</tr>
<tr>
<td>113</td>
<td>(\text{C}_6\text{H}_12\text{O}_6\text{(cr) 3rd law entropy of glucose(cr. Based on data of Simon (1922) Assumed to be a form})</td>
<td>S</td>
<td>211.3</td>
<td>10.0</td>
<td>0.000</td>
<td>29PAR/KEL</td>
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<td>No.</td>
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<td>Property</td>
<td>Observed $\Delta H_{\text{meas}}$</td>
<td>Unc. $\Delta H_{\text{meas}}$</td>
<td>Residual</td>
<td>Reference</td>
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<tr>
<td>111</td>
<td>C$<em>6$H$</em>{12}$O$_6$(cr5)</td>
<td>S</td>
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<td>C$<em>6$H$</em>{12}$O$_6$(cr3) $+ 5$ O$_2$(g) $= 5$ CO$_2$(g) $+ 5$ H$_2$O(l)</td>
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<td>C$<em>6$H$</em>{12}$O$_6$(cr) $+ 6$ O$_2$(g) $= 6$ CO$_2$(g) $+ 6$ H$_2$O(l)</td>
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Table 11. Catalog of thermochemical measurements at 298.15 K: equilibrium, enthalpy, and entropy data — Continued
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<th>No.</th>
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<th>Property</th>
<th>Observed $\Delta H$ (kJ mol$^{-1}$)</th>
<th>Unc. (J mol$^{-1}$ K$^{-1}$)</th>
<th>Residual</th>
<th>Reference</th>
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<td>C$<em>7$H$</em>{12}$O$_4$(cr4) + 6 O$_2$(g) = 6 CO$_2$(g) + 6 H$_2$O(l)</td>
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<td>C$<em>7$H$</em>{12}$O$_5$(cr5) + 6 O$_2$(g) = 6 CO$_2$(g) + 6 H$_2$O(l)</td>
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<td>C$<em>7$H$</em>{12}$O$_5$(cr) = C$<em>7$H$</em>{12}$O$_5$(ao)</td>
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<td>C$<em>6$H$</em>{12}$O$_6$(cr2) = C$<em>6$H$</em>{12}$O$_6$(ao)</td>
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<td>C$<em>6$H$</em>{12}$O$_6$(cr) = C$<em>6$H$</em>{12}$O$_6$(ao) + H$_2$O(l)</td>
<td>$\Delta H$</td>
<td>20.9</td>
<td>1.0</td>
<td>0.027</td>
<td>97BRO/PIE</td>
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<tr>
<td></td>
<td>Enthalpy of solution of glucose monohydrate</td>
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<td>No.</td>
<td>Reaction</td>
<td>Property</td>
<td>Observed $\Delta H$ (kJ mol$^{-1}$)</td>
<td>Unc. $\Delta H$ (kJ mol$^{-1}$)</td>
<td>Residual $\Delta H$ (kJ mol$^{-1}$)</td>
<td>Reference</td>
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<tr>
<td>51</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{cr}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao}) - \text{H}_2\text{O}(l)$</td>
<td>$\Delta H$</td>
<td>20.9</td>
<td>0.5</td>
<td>0.027</td>
<td>34HEN/STE</td>
</tr>
<tr>
<td>52</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{cr}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao}) - \text{H}_2\text{O}(l)$</td>
<td>$\Delta H$</td>
<td>20.34</td>
<td>0.40</td>
<td>-0.033</td>
<td>55TAY/ROW</td>
</tr>
<tr>
<td>53</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{cr8}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao})$</td>
<td>$\Delta H$</td>
<td>4.4</td>
<td>0.5</td>
<td>0.000</td>
<td>46ROW/PAR</td>
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<td>54</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{cr4}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao2})$</td>
<td>$\Delta H$</td>
<td>6.85</td>
<td>0.50</td>
<td>-1.010</td>
<td>82JAS/AHL</td>
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<tr>
<td>55</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{cr4}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao2})$</td>
<td>$\Delta H$</td>
<td>7.87</td>
<td>0.30</td>
<td>0.000</td>
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</tr>
<tr>
<td>56</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{cr5}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao4})$</td>
<td>$\Delta H$</td>
<td>16.45</td>
<td>0.50</td>
<td>-0.687</td>
<td>34HEN/STE</td>
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<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{cr5}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao4})$</td>
<td>$\Delta H$</td>
<td>17.20</td>
<td>0.50</td>
<td>0.063</td>
<td>82JAS/AHL</td>
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<td>58</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{cr5}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao4})$</td>
<td>$\Delta H$</td>
<td>17.10</td>
<td>0.30</td>
<td>-0.037</td>
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<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{cr6}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao3})$</td>
<td>$\Delta H$</td>
<td>9.4</td>
<td>2.0</td>
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<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{cr6}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao3})$</td>
<td>$\Delta H$</td>
<td>9.05</td>
<td>1.00</td>
<td>-1.030</td>
<td>34HEN/STE</td>
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<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{cr6}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao3})$</td>
<td>$\Delta H$</td>
<td>8.83</td>
<td>1.00</td>
<td>-1.280</td>
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<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{cr6}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{ao3})$</td>
<td>$\Delta H$</td>
<td>10.38</td>
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<td>kJ mol⁻¹</td>
<td>J mol⁻¹ K⁻¹</td>
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<tr>
<td>153</td>
<td>C₄H₁₀O₄(cr,7) = C₄H₇O₄(aq5) Enthalpy of solution of sorbose</td>
<td>ΔH</td>
<td>6.94</td>
<td>0.50</td>
<td>0.000</td>
<td>82JAS/AHL</td>
</tr>
<tr>
<td>154</td>
<td>C₄H₁₀O₄(cr) = C₄H₇O₄(aq) + H₂O(l) Gibbs energy of solution of α-glucose monohydrate Use solubility of 4.55 mol kg⁻¹, γ of 1.21, a(H₂O) = 0.889 Listed for information only</td>
<td>ΔG</td>
<td>-4.0</td>
<td>0.5</td>
<td>0.741</td>
<td>17DEH</td>
</tr>
<tr>
<td>155</td>
<td>C₄H₁₀O₄(cr) = C₄H₇O₄(aq) + H₂O(l) Gibbs energy of solution of α-glucose monohydrate Use solubility of 5.89 mol kg⁻¹, γ of 1.25, a(H₂O) = 0.889</td>
<td>ΔG</td>
<td>-4.74</td>
<td>0.20</td>
<td>0.001</td>
<td>22JAC/SIL</td>
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<td>156</td>
<td>C₄H₁₀O₄(cr) = C₄H₇O₄(aq) + H₂O(l) Gibbs energy of solution of α-glucose monohydrate Use solubility of 5.75 mol kg⁻¹, γ of 1.23, a(H₂O) = 0.889</td>
<td>ΔG</td>
<td>-4.68</td>
<td>0.50</td>
<td>0.061</td>
<td>23GIL</td>
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<td>157</td>
<td>C₄H₁₀O₄(cr) = C₄H₇O₄(aq) + H₂O(l) Gibbs energy of solution of α-glucose monohydrate Use solubility of 5.63 mol kg⁻¹, γ of 1.38, a(H₂O) = 0.889</td>
<td>ΔG</td>
<td>-4.79</td>
<td>0.40</td>
<td>-0.049</td>
<td>52TAL/HUN</td>
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<td>158</td>
<td>C₄H₁₀O₄(cr) = C₄H₇O₄(aq) Gibbs energy of solution of glucose (anhydrous) Assumed to be α form Uses solubility of 11.27 and γ of 1.56</td>
<td>ΔG</td>
<td>-7.11</td>
<td>0.50</td>
<td>0.000</td>
<td>22JAC/SIL</td>
</tr>
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<td>159</td>
<td>C₄H₁₀O₄(cr) = C₄H₇O₄(aq) Gibbs energy of solution of galactose Use solubility of 3.79 mol kg⁻¹ and γ of 1.17 Listed for information only</td>
<td>ΔG</td>
<td>-3.69</td>
<td>0.50</td>
<td>-1.090</td>
<td>17DEH</td>
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<td>160</td>
<td>C₄H₁₀O₄(cr) = C₄H₇O₄(aq) Gibbs energy of solution of galactose Use solubility of 2.62 mol kg⁻¹ and γ of 1.10 Assumes that solid phase is anhydrous</td>
<td>ΔG</td>
<td>-2.60</td>
<td>0.50</td>
<td>0.000</td>
<td>40GOU</td>
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<td>161</td>
<td>C₄H₁₀O₄(cr) = C₄H₇O₄(aq) Gibbs energy of solution of galactose Use solubility of 2.62 mol kg⁻¹ and γ of 1.10 Assumes that solid phase is anhydrous</td>
<td>ΔG</td>
<td>-2.6</td>
<td>0.5</td>
<td>0.000</td>
<td>52TAL/HUN</td>
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<td>162</td>
<td>C₄H₁₀O₄(cr) = C₄H₇O₄(aq) Gibbs energy of solution of fructose Use solubility of 22.59 mol kg⁻¹ and γ of 2.3</td>
<td>ΔG</td>
<td>-5.8</td>
<td>0.5</td>
<td>0.067</td>
<td>26JAC/SIL</td>
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<tr>
<td>No.</td>
<td>Reaction</td>
<td>Property</td>
<td>Observed $\Delta G$ (kJ mol$^{-1}$)</td>
<td>Unc. $\Delta G$ (kJ mol$^{-1}$)</td>
<td>Residual</td>
<td>Reference</td>
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<tr>
<td>173</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6$ (cr6) = $\text{C}<em>6\text{H}</em>{12}\text{O}_6$ (aq3)</td>
<td>$\Delta G$</td>
<td>-12.0</td>
<td>1.0</td>
<td>-0.133</td>
<td>52YOU/JOH</td>
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<tr>
<td></td>
<td>Gibbs energy of solution of fructose</td>
<td>Use solubility of 23.26 mol kg$^{-1}$ and $\gamma$ of 2.4</td>
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<tr>
<td>174</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6$ (cr) = $\text{C}<em>6\text{H}</em>{12}\text{O}_6$ (aq3) + 0.5 $\text{H}_2\text{O}$ (l)</td>
<td>$\Delta G$</td>
<td>-12.0</td>
<td>1.0</td>
<td>0.000</td>
<td>52YOU/JOH</td>
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<td>Gibbs energy of solution of fructose hemihydrate</td>
<td>Use soln. of 23.91 mol kg$^{-1}$, $\alpha$(H$_2$O) = 1.0 and $\gamma$ of 24</td>
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<td>175</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6$ (cr7) = $\text{C}<em>6\text{H}</em>{12}\text{O}_6$ (aq5)</td>
<td>$\Delta G$</td>
<td>-3.1</td>
<td>0.5</td>
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<td>00LOB/ERE</td>
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<td>Gibbs energy of solution of sorbose</td>
<td>Use solubility of 3.08 mol kg$^{-1}$ and $\gamma$ of 1.13</td>
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<td>Assumes that solid phase is anhydrous</td>
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<td>176</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6$ (cr4) = $\text{C}<em>6\text{H}</em>{12}\text{O}_6$ (aq2)</td>
<td>$\Delta G$</td>
<td>-8.8</td>
<td>0.5</td>
<td>0.000</td>
<td>88TEW/GOL</td>
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<td>Gibbs energy of solution of mannose</td>
<td>Use solubility of 17.3 mol kg$^{-1}$ and $\gamma$ of 2.0</td>
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<td>Assumes that solid phase is anhydrous</td>
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<td>177</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6$ (cr4) = $\text{C}<em>6\text{H}</em>{12}\text{O}_6$ (ao)</td>
<td>$\Delta G$</td>
<td>-8.7</td>
<td>0.5</td>
<td>0.000</td>
<td>88TEW/GOL</td>
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<td>Gibbs energy of solution of ribose</td>
<td>Use solubility of 20.0 mol kg$^{-1}$ and $\gamma$ of 1.7</td>
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<td>Assumes that solid phase is anhydrous</td>
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<td>178</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6$ (cr3) = $\text{C}<em>6\text{H}</em>{12}\text{O}_6$ (ao3)</td>
<td>$\Delta G$</td>
<td>-5.9</td>
<td>0.5</td>
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<td>88TEW/GOL</td>
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<td>Gibbs energy of solution of xylene</td>
<td>Use solubility of 3.3 mol kg$^{-1}$ and $\gamma$ of 0.28</td>
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<td>Assumes that solid phase is anhydrous</td>
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<td>179</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6$ (cr2) = $\text{C}<em>6\text{H}</em>{12}\text{O}_6$ (ao5)</td>
<td>$\Delta G$</td>
<td>-4.5</td>
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<td>88TEW/GOL</td>
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<td>Gibbs energy of solution of xylobose</td>
<td>Use solubility of 3.17 mol kg$^{-1}$ and $\gamma$ of 1.18</td>
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<td>Assumes that solid phase is anhydrous</td>
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<td>180</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6$ (cr4) = $\text{C}<em>6\text{H}</em>{12}\text{O}_6$ (ao8)</td>
<td>$\Delta G$</td>
<td>-8.3</td>
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<td>Use solubility of 17.84 mol kg$^{-1}$ and $\gamma$ of 1.6</td>
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<td>Assumes that solid phase is anhydrous</td>
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<td>No.</td>
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<tr>
<td>81</td>
<td>(C_6H_{12}O_6^{(ao)} = C_6H_{12}O_6^{(ao)} + H^+(ao))</td>
<td>(\Delta G)</td>
<td>6975</td>
<td>0.50</td>
<td>0.630</td>
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<td>82</td>
<td>(C_6H_{12}O_6^{(ao)} = C_6H_{12}O_6^{(ao)} + H^+(ao))</td>
<td>(\Delta G)</td>
<td>6912</td>
<td>0.20</td>
<td>0.000</td>
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<td>(C_6H_{12}O_6^{(ao)} = C_6H_{12}O_6^{(ao)} + H^+(ao))</td>
<td>(\Delta H)</td>
<td>3389</td>
<td>1.00</td>
<td>-2.210</td>
<td>66IZA/RYT</td>
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<td>(C_6H_{12}O_6^{(ao)} = C_6H_{12}O_6^{(ao)} + H^+(ao))</td>
<td>(\Delta H)</td>
<td>361</td>
<td>0.5</td>
<td>0.000</td>
<td>70CHR/RYT</td>
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<td>85</td>
<td>(C_6H_{12}O_6^{(ao3)} = C_6H_{12}O_6^{(ao3)} + H^+(ao))</td>
<td>(\Delta G)</td>
<td>692</td>
<td>0.5</td>
<td>-0.200</td>
<td>00OSA</td>
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<td>1st ionization of xylose</td>
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<td>Adjusted to 298.15 K using (\Delta H = 37.7) kJ mol(^{-1})</td>
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<td>The ionic strength was not specified by the authors</td>
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<td>86</td>
<td>(C_6H_{12}O_6^{(ao3)} = C_6H_{12}O_6^{(ao3)} + H^+(ao))</td>
<td>(\Delta G)</td>
<td>692</td>
<td>0.5</td>
<td>-0.200</td>
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<td>1st ionization of xylose</td>
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<td>Adjusted to 298.15 K using (\Delta H = 37.7) kJ mol(^{-1})</td>
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<td>Adjusted to zero ionic strength using (B = 1.6) kg mol(^{-1})</td>
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<td>87</td>
<td>(C_6H_{12}O_6^{(ao3)} = C_6H_{12}O_6^{(ao3)} + H^+(ao))</td>
<td>(\Delta G)</td>
<td>673</td>
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<td>88</td>
<td>(C_6H_{12}O_6^{(ao3)} = C_6H_{12}O_6^{(ao3)} + H^+(ao))</td>
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<td>702</td>
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<td>(C_6H_{12}O_6^{(ao3)} = C_6H_{12}O_6^{(ao3)} + H^+(ao))</td>
<td>(\Delta G)</td>
<td>69</td>
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<td>(C_6H_{12}O_6^{(ao3)} = C_6H_{12}O_6^{(ao3)} + H^+(ao))</td>
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<td>(C_6H_{12}O_6^{(ao3)} = C_6H_{12}O_6^{(ao3)} + H^+(ao))</td>
<td>(\Delta H)</td>
<td>37.1</td>
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<td>$\text{C}_6\text{H}_5\text{O}_5\text{(ao3)} = \text{C}_6\text{H}_5\text{O}_6^-(\text{ao3}) + \text{H}^+(\text{ao})$</td>
<td>$\Delta G$</td>
<td>81.63</td>
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<td>$\text{C}_6\text{H}_5\text{O}_5\text{(ao5)} = \text{C}_6\text{H}_5\text{O}_6^-(\text{ao5}) + \text{H}^+(\text{ao})$</td>
<td>$\Delta G$</td>
<td>71.20</td>
<td>0.50</td>
<td>0.760</td>
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<td>$\Delta G$</td>
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<td>$\Delta G$</td>
<td>70.44</td>
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<td>$\Delta H$</td>
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<td>$\text{C}_6\text{H}_5\text{O}_5\text{(ao5)} = \text{C}_6\text{H}_5\text{O}_6^-(\text{ao5}) + \text{H}^+(\text{ao})$</td>
<td>$\Delta H$</td>
<td>40.0</td>
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<td>0.000</td>
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<td>201</td>
<td>C₆H₅O₂⁺(ao5) + H⁺(ao)</td>
<td>ΔG</td>
<td>84.02</td>
<td>1.00</td>
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<td>202</td>
<td>C₆H₅O₂⁺(ao8) = C₆H₅O₂⁺(ao8) - H⁺(ao)</td>
<td>ΔG</td>
<td>69.12</td>
<td>0.50</td>
<td>0.00</td>
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<td>203</td>
<td>C₆H₅O₂⁺(ao8) = C₆H₅O₂⁺(ao8) - H⁺(ao)</td>
<td>ΔG</td>
<td>69.12</td>
<td>0.20</td>
<td>0.00</td>
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<td>204</td>
<td>C₆H₅O₂⁺(ao8) = C₆H₅O₂⁺(ao8) - H⁺(ao)</td>
<td>ΔH</td>
<td>33.47</td>
<td>1.00</td>
<td>0.00</td>
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<td>205</td>
<td>C₆H₅O₂⁺(ao8) = C₆H₅O₂⁺(ao8) - H⁺(ao)</td>
<td>ΔH</td>
<td>33.5</td>
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<td>C₆H₅O₂⁺(ao) = C₆H₅O₂⁺(ao) + H⁺(ao)</td>
<td>ΔG</td>
<td>69.18</td>
<td>0.50</td>
<td>-3.920</td>
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<td>Adjusted to 298.15 K using ΔH = 36.7 kJ mol⁻¹</td>
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<td>C₆H₅O₂⁺(ao) = C₆H₅O₂⁺(ao) + H⁺(ao)</td>
<td>ΔG</td>
<td>70.39</td>
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<td>208</td>
<td>C₆H₅O₂⁺(ao) = C₆H₅O₂⁺(ao) + H⁺(ao)</td>
<td>ΔG</td>
<td>69.85</td>
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<td>C₆H₅O₂⁺(ao) = C₆H₅O₂⁺(ao) + H⁺(ao)</td>
<td>ΔG</td>
<td>69.85</td>
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<td>210</td>
<td>( C_6H_{12}O_6^{(a)} = C_6H_{11}O_5^{(a)} + H^+(a) )</td>
<td>( \Delta G )</td>
<td>68.58 0.50</td>
<td>-1.120</td>
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<td>( C_6H_{12}O_6^{(a)} = C_6H_{11}O_5^{(a)} + H^+(a) )</td>
<td>( \Delta G )</td>
<td>70.5 0.50</td>
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<td>212</td>
<td>( C_6H_{12}O_6^{(a)} = C_6H_{11}O_5^{(a)} + H^+(a) )</td>
<td>( \Delta G )</td>
<td>70.2 0.50</td>
<td>0.620</td>
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<td>Adjusted to zero ionic strength using ( B = 1.6 \text{ kg mol}^{-1} )</td>
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<td>Adjusted to 298.15 K using ( \Delta H = 36.7 \text{ kJ mol}^{-1} )</td>
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<td>213</td>
<td>( C_6H_{12}O_6^{(a)} = C_6H_{11}O_5^{(a)} + H^+(a) )</td>
<td>( \Delta G )</td>
<td>70.7 0.5</td>
<td>0.600</td>
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<td>214</td>
<td>( C_6H_{12}O_6^{(a)} = C_6H_{11}O_5^{(a)} + H^+(a) )</td>
<td>( \Delta G )</td>
<td>68.2 0.5</td>
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<td>50SOU/SCH</td>
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<td>215</td>
<td>( C_6H_{12}O_6^{(a)} = C_6H_{11}O_5^{(a)} - H^+(a) )</td>
<td>( \Delta G )</td>
<td>71.3 0.5</td>
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<td>Adjusted to 298.15 K using ( \Delta H = 36.7 \text{ kJ mol}^{-1} )</td>
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<td>Adjusted to zero ionic strength using ( B = 1.6 \text{ kg mol}^{-1} )</td>
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<td>Listed for information only</td>
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<tr>
<td>216</td>
<td>( C_6H_{12}O_6^{(a)} = C_6H_{11}O_5^{(a)} - H^+(a) )</td>
<td>( \Delta G )</td>
<td>71.4 0.50</td>
<td>1.300</td>
<td>53KIL/WYN</td>
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<td>1st ionization of glucose</td>
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<td>Adjusted to zero ionic strength using ( B = 1.6 \text{ kg mol}^{-1} )</td>
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<td>217</td>
<td>( C_6H_{12}O_6^{(a)} = C_6H_{11}O_5^{(a)} - H^+(a) )</td>
<td>( \Delta G )</td>
<td>68.3 0.5</td>
<td>-1.800</td>
<td>55SCH</td>
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<td>The temperature and ionic strength were not specified by the authors</td>
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<tr>
<td>No.</td>
<td>Reaction</td>
<td>Property</td>
<td>Observed ( \Delta G )</td>
<td>Unc. ( \Delta G )</td>
<td>Residual</td>
<td>Reference</td>
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<tr>
<td>218</td>
<td>( \text{C}<em>6\text{H}</em>{12}\text{O}_6\text{(ao)} = \text{C}<em>6\text{H}</em>{11}\text{O}_7\text{(ao)} + \text{H}^+\text{(ao)} )</td>
<td>( \Delta G )</td>
<td>70.3</td>
<td>0.5</td>
<td>2.200</td>
<td>57LOS/SIM</td>
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<tr>
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<td>1st ionization of glucose</td>
<td>Listed for information only</td>
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<td>219</td>
<td>( \text{C}<em>6\text{H}</em>{12}\text{O}_6\text{(ao)} = \text{C}<em>6\text{H}</em>{11}\text{O}_7\text{(ao)} + \text{H}^+\text{(ao)} )</td>
<td>( \Delta G )</td>
<td>74.7</td>
<td>0.5</td>
<td>4.600</td>
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<td>Adjusted to zero ionic strength using ( B = 1.6 ) ( \text{kg mol}^{-1} )</td>
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<td>220</td>
<td>( \text{C}<em>6\text{H}</em>{12}\text{O}_6\text{(ao)} = \text{C}<em>6\text{H}</em>{11}\text{O}_7\text{(ao)} + \text{H}^+\text{(ao)} )</td>
<td>( \Delta G )</td>
<td>70.5</td>
<td>0.5</td>
<td>3.400</td>
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<td>1st ionization of glucose</td>
<td>Assumed to be at zero ionic strength</td>
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<td>221</td>
<td>( \text{C}<em>6\text{H}</em>{12}\text{O}_6\text{(ao)} = \text{C}<em>6\text{H}</em>{11}\text{O}_7\text{(ao)} + \text{H}^+\text{(ao)} )</td>
<td>( \Delta G )</td>
<td>71.2</td>
<td>0.5</td>
<td>1.100</td>
<td>66IZA/RYT</td>
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<td>1st ionization of glucose</td>
<td>Listed for information only</td>
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<td>222</td>
<td>( \text{C}<em>6\text{H}</em>{12}\text{O}_6\text{(ao)} = \text{C}<em>6\text{H}</em>{11}\text{O}_7\text{(ao)} + \text{H}^+\text{(ao)} )</td>
<td>( \Delta G )</td>
<td>70.1</td>
<td>0.5</td>
<td>2.000</td>
<td>70CHR/RYT</td>
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<td>1st ionization of glucose</td>
<td>Listed for information only</td>
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<td>223</td>
<td>( \text{C}<em>6\text{H}</em>{12}\text{O}_6\text{(ao)} = \text{C}<em>6\text{H}</em>{11}\text{O}_7\text{(ao)} + \text{H}^+\text{(ao)} )</td>
<td>( \Delta H )</td>
<td>30.5</td>
<td>3.0</td>
<td>-6.200</td>
<td>53KIL/WYN</td>
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<td>1st ionization of glucose</td>
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<td>224</td>
<td>( \text{C}<em>6\text{H}</em>{12}\text{O}_6\text{(ao)} = \text{C}<em>6\text{H}</em>{11}\text{O}_7\text{(ao)} + \text{H}^+\text{(ao)} )</td>
<td>( \Delta H )</td>
<td>41.8</td>
<td>3.0</td>
<td>5.100</td>
<td>57LOS/SIM</td>
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<td>225</td>
<td>( \text{C}<em>6\text{H}</em>{12}\text{O}_6\text{(ao)} = \text{C}<em>6\text{H}</em>{11}\text{O}_7\text{(ao)} + \text{H}^+\text{(ao)} )</td>
<td>( \Delta H )</td>
<td>32.2</td>
<td>1.0</td>
<td>-4.500</td>
<td>66IZA/RYT</td>
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<td>1st ionization of glucose</td>
<td>Listed for information only</td>
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<td>226</td>
<td>( \text{C}<em>6\text{H}</em>{12}\text{O}_6\text{(ao)} = \text{C}<em>6\text{H}</em>{11}\text{O}_7\text{(ao)} + \text{H}^+\text{(ao)} )</td>
<td>( \Delta H )</td>
<td>36.7</td>
<td>0.5</td>
<td>2.000</td>
<td>70CHR/RYT</td>
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<td>1st ionization of glucose</td>
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<td>227</td>
<td>( \text{C}<em>6\text{H}</em>{12}\text{O}_6\text{(ao)} = \text{C}<em>6\text{H}</em>{11}\text{O}_7\text{(ao)} + \text{H}^+\text{(ao)} )</td>
<td>( \Delta G )</td>
<td>77.2</td>
<td>1.0</td>
<td>-3.850</td>
<td>29HIR/SCH</td>
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<td>2nd ionization of glucose</td>
<td>Adjusted to zero ionic strength using ( E = 1.6 ) ( \text{kg mol}^{-1} )</td>
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<tr>
<td>No.</td>
<td>Reaction</td>
<td>Property</td>
<td>Observed $\Delta G$ (kJ mol$^{-1}$ or J mol$^{-1}$ K$^{-1}$)</td>
<td>Unc.</td>
<td>Residual</td>
<td>Reference</td>
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<tr>
<td>228</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6^{+}(\text{aq}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6\text{O}^-\text{aq}) + \text{H}^+\text{aq})$</td>
<td>$\Delta G$</td>
<td>81.2</td>
<td>1.0</td>
<td>0.250</td>
<td>31STE</td>
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<td>2nd ionization of glucose</td>
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<td></td>
<td>Adjusted to zero ionic strength using $B = 1.6$ kg$^2$ mol$^{-1}$</td>
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<td></td>
<td>Adjusted to 298.15 K using $\Delta H = 36.7$ kJ mol$^{-1}$</td>
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<td>229</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6^{+}(\text{aq}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6\text{O}^-\text{aq}) + \text{H}^+\text{aq})$</td>
<td>$\Delta G$</td>
<td>82.2</td>
<td>1.0</td>
<td>1.450</td>
<td>32URB/SHA</td>
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<td>2nd ionization of glucose</td>
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<td></td>
<td>Adjusted to zero ionic strength using $B = 1.6$ kg$^2$ mol$^{-1}$</td>
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<tr>
<td>230</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6^{+}(\text{aq}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6\text{O}^-\text{aq}) + \text{H}^+\text{aq})$</td>
<td>$\Delta G$</td>
<td>80.2</td>
<td>1.0</td>
<td>-0.850</td>
<td>50SOU/SCH</td>
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<td>2nd ionization of glucose</td>
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<td>The temperature and ionic strength were not specified by the authors</td>
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<td>231</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6^{+}(\text{aq}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6\text{O}^-\text{aq}) + \text{H}^+\text{aq})$</td>
<td>$\Delta G$</td>
<td>80.2</td>
<td>1.0</td>
<td>-0.850</td>
<td>55SCH</td>
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<tr>
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<td>2nd ionization of glucose</td>
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<td>The temperature and ionic strength were not specified by the authors</td>
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<td>232</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6^{+}(\text{aq}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6\text{O}^-\text{aq}) + \text{H}^+\text{aq})$</td>
<td>$\Delta G$</td>
<td>85.3</td>
<td>1.0</td>
<td>0.000</td>
<td>31STE</td>
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<td>3rd ionization of glucose</td>
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<td>Adjusted to zero ionic strength using $B = 1.6$ kg$^2$ mol$^{-1}$</td>
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<td>Adjusted to 298.15 K using $\Delta H = 36.7$ kJ mol$^{-1}$</td>
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<td>233</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6^{+}(\text{aq}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6\text{O}^-\text{aq}) + \text{H}^+\text{aq})$</td>
<td>$\Delta G$</td>
<td>86.3</td>
<td>1.0</td>
<td>0.000</td>
<td>31STE</td>
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<td>4th ionization of glucose</td>
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<td>Adjusted to zero ionic strength using $B = 1.6$ kg$^2$ mol$^{-1}$</td>
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<td>Adjusted to 298.15 K using $\Delta H = 36.7$ kJ mol$^{-1}$</td>
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<td>234</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{aq2}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{aq2}) + \text{H}^+\text{aq})$</td>
<td>$\Delta G$</td>
<td>74.4</td>
<td>0.5</td>
<td>5.450</td>
<td>13MIC</td>
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<td>1st ionization of mannose</td>
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<td>Adjusted to 298.15 K using $\Delta H = 33.1$ kJ mol$^{-1}$</td>
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<td>Adjusted to zero ionic strength using $B = 1.6$ kg$^2$ mol$^{-1}$</td>
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<td>235</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{aq2}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{aq2}) + \text{H}^+\text{aq})$</td>
<td>$\Delta G$</td>
<td>74.9</td>
<td>0.50</td>
<td>5.440</td>
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<td>Adjusted to 298.15 K using $\Delta H = 33.1$ kJ mol$^{-1}$</td>
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<td>Adjusted to zero ionic strength using $B = 1.6$ kg$^2$ mol$^{-1}$</td>
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<tr>
<td>236</td>
<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{aq2}) = \text{C}<em>6\text{H}</em>{12}\text{O}_6(\text{aq2}) + \text{H}^+\text{aq})$</td>
<td>$\Delta G$</td>
<td>67.7</td>
<td>0.50</td>
<td>-1.480</td>
<td>55SCH</td>
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<td>1st ionization of mannose</td>
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<td>The temperature and ionic strength were not specified by the authors</td>
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<tr>
<td>No.</td>
<td>Reaction</td>
<td>Property</td>
<td>Observed $\Delta H$ or $\Delta G$</td>
<td>Unc. $\Delta H$ or $\Delta G$</td>
<td>Residual $\Delta H$ or $\Delta G$</td>
<td>Reference</td>
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<tr>
<td>237</td>
<td>$C_6H_{12}O_6(aq 02) = C_6H_{13}O_6^-(aq 02) + H^+(aq)$</td>
<td>$\Delta G$</td>
<td>68.95</td>
<td>0.20</td>
<td>0.000</td>
<td>66IZA/RYT</td>
</tr>
<tr>
<td>238</td>
<td>$C_6H_{12}O_6(aq 02) = C_6H_{13}O_6^-(aq 02) + H^+(aq)$</td>
<td>$\Delta G$</td>
<td>68.95</td>
<td>0.20</td>
<td>0.000</td>
<td>70CHR/RYT</td>
</tr>
<tr>
<td>239</td>
<td>$C_6H_{12}O_6(aq 02) = C_6H_{13}O_6^-(aq 02) + H^+(aq)$</td>
<td>$\Delta H$</td>
<td>33.05</td>
<td>0.50</td>
<td>$-0.025$</td>
<td>66IZA/RYT</td>
</tr>
<tr>
<td>240</td>
<td>$C_6H_{12}O_6(aq 02) = C_6H_{13}O_6^-(aq 02) + H^+(aq)$</td>
<td>$\Delta H$</td>
<td>33.1</td>
<td>0.5</td>
<td>0.025</td>
<td>70CHR/RYT</td>
</tr>
<tr>
<td>241</td>
<td>$C_6H_{12}O_6^-(aq 02) = C_6H_{13}O_6^-\cdot(aq 02) + H^+-\cdot(aq 02)$</td>
<td>$\Delta G$</td>
<td>80.8</td>
<td>1.0</td>
<td>0.000</td>
<td>55SCH</td>
</tr>
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</table>

2nd ionization of mannose
The temperature and ionic strength were not specified by the authors

| 242 | $C_6H_{12}O_6(aq 03) = C_6H_{13}O_6^+(aq 03) + H^+(aq)$ | $\Delta G$ | 72.8 | 0.5 | 4.100 | 00OSA |

1st ionization of fructose
Adjusted to 298 K using $\Delta H = 39.2 \text{ kJ mol}^{-1}$
The ionic strength was not specified by the authors
Listed for information only

| 243 | $C_6H_{12}O_6(aq 03) = C_6H_{13}O_6^+(aq 03) + H^+(aq)$ | $\Delta G$ | 69.2 | 0.5 | 0.500 | 01MAD |

1st ionization of fructose
Adjusted to 298 K using $\Delta H = +31.7 \text{ kJ mol}^{-1}$
Listed for information only

| 244 | $C_6H_{12}O_6(aq 03) = C_6H_{13}O_6^+(aq 03) + H^+(aq)$ | $\Delta G$ | 69.1 | 0.5 | 0.400 | 13MIC |

1st ionization of fructose
Adjusted to 298 K using $\Delta H = 39.2 \text{ kJ mol}^{-1}$
Adjusted to zero ionic strength using $I = 1.6 \text{ kg mol}^{-1}$
Listed for information only

| 245 | $C_6H_{12}O_6(aq 03) = C_6H_{13}O_6^+(aq 03) + H^+(aq)$ | $\Delta G$ | 69.1 | 0.5 | 0.400 | 13MIC/RON |

1st ionization of fructose
Adjusted to 298 K using $\Delta H = 39.2 \text{ kJ mol}^{-1}$
Adjusted to zero ionic strength using $I = 1.6 \text{ kg mol}^{-1}$
Listed for information only

| 246 | $C_6H_{12}O_6(aq 03) = C_6H_{13}O_6^+(aq 03) + H^+(aq)$ | $\Delta G$ | 68.35 | 0.50 | $-0.350$ | 29HRI/SCH |

1st ionization of fructose
Adjusted to zero ionic strength using $I = 1.6 \text{ kg mol}^{-1}$
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<table>
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<th>No.</th>
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<th>Observed, $\Delta G$ (kJ mol$^{-1}$)</th>
<th>Unc., $\Delta H$ (kJ mol$^{-1}$)</th>
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<td>$\text{C}<em>6\text{H}</em>{12}\text{O}_6\text{(aq3)} = \text{C}<em>6\text{H}</em>{12}\text{O}_6\text{(aq3)} + \text{H}^+(\text{aq})$</td>
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<td>C₂H₇O₂⁻(ao4) = C₂H₇O₂⁻(ao4) + H⁺(ao)</td>
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<td>67.2</td>
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<td>C₂H₇O₂⁻(ao4) = C₂H₇O₂⁻(ao4) + H⁺(ao)</td>
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<td>$\text{C}_3\text{H}_7\text{O}_4(\text{aq}) = C_6\text{H}_5\text{O}_4^-(\text{aq}) + H^+(\text{aq})$</td>
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### Table 11. Catalog of Thermochemical Measurements at 298.15 K: equilibrium, enthalpy, and entropy data — Continued

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<td>( C_4H_8O_5P^- (aq) = C_4H_6O_5P^2^- (aq) + F^+ (aq) ) 2nd ionization of ribose-5P</td>
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<td>$C_6H_{12}O_5^{2-}(\text{ao}) = C_6H_{12}O_5^{2+}(\text{ao}) + H^+(\text{ao})$</td>
<td>2nd ionization of glucose-4P</td>
<td>$33.4$</td>
<td>$0.5$</td>
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<td>$C_6H_{12}O_5^{2+}(\text{ao}) = C_6H_{12}O_5^{2+}(\text{ao}) + H^+(\text{ao})$</td>
<td>2nd ionization of glucose-4P</td>
<td>$35.8$</td>
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<td>66BUN/CHA</td>
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<td>302</td>
<td>$C_6H_{12}O_5^{2+}(\text{ao}) = C_6H_{12}O_5^{2+}(\text{ao}) + H^+(\text{ao})$</td>
<td>2nd ionization of glucose-4P</td>
<td>$35.5$</td>
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<td>$C_6H_{12}O_5^{2+}(\text{ao}) = C_6H_{12}O_5^{2+}(\text{ao}) + H^+(\text{ao})$</td>
<td>3rd ionization of glucose-6P</td>
<td>$65.8$</td>
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<td>$C_6H_{12}O_5^{2+}(\text{ao}) = C_6H_{12}O_5^{2+}(\text{ao}) + H^+(\text{ao})$</td>
<td>3rd ionization of glucose-6P</td>
<td>$35.2$</td>
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<td>305</td>
<td>$C_6H_{12}O_5^{2+}(\text{ao4}) = C_6H_{12}O_5^{2+}(\text{ao4}) + H^+(\text{ao})$</td>
<td>2nd ionization of fructose-5P</td>
<td>$35.8$</td>
<td>$0.3$</td>
<td>$0.000$</td>
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<td>306</td>
<td>CaC₆H₁₂O₇P(aq4) = C₆H₁₂O₇P²⁻(aq4) + Ca²⁺(aq)</td>
<td>( \Delta G )</td>
<td>13.4</td>
<td>0.3</td>
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<td>Dissociation of C₆-fructose-6P</td>
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<td>307</td>
<td>MgC₆H₁₂O₇P(aq4) = C₆H₁₂O₇P²⁻(aq4) + Mg²⁺(aq)</td>
<td>( \Delta G )</td>
<td>14.1</td>
<td>0.3</td>
<td>0000</td>
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<td>Dissociation of Mg-fructose-6P</td>
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<td>Adjusted to zero ionic strength using ( B = 1.6 \text{ kg} \text{l mol}^{-1} )</td>
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<td>308</td>
<td>C₆H₁₂O₇P(aq6) = C₆H₁₂O₇P²⁻(aq6) + H⁺(aq)</td>
<td>( \Delta G )</td>
<td>6.96</td>
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<td>1st ionization of galactose-1P</td>
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<td>Adjusted to zero ionic strength using ( B = 1.6 \text{ kg} \text{l mol}^{-1} )</td>
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<td>Adjusted to 298.15 K using ( \Delta H = -1.8 \text{ kJ mol}^{-1} )</td>
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<tr>
<td>309</td>
<td>C₆H₁₂O₇P²⁻(aq6) = C₆H₁₂O₇P²⁻(aq6) + H⁺(aq)</td>
<td>( \Delta G )</td>
<td>37.7</td>
<td>0.3</td>
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<td>2nd ionization of galactose-1P</td>
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<td>Adjusted to zero ionic strength using ( B = 1.6 \text{ kg} \text{l mol}^{-1} )</td>
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</table>

3.2.5.3 These reactions, with the property type "HGS", represent the constraint \( \Delta G^\circ - \Delta G^\bullet + T\Delta S^\circ = 0 \) for the formation of individual substance. As an example, reaction 310 is given below. [85GAR/PAR]

| 310 | sec-PrOH = PrOH + 5.5H₂(g) + 4.5O₂(g) = C₆H₁₂O₇P²⁻(aq) | HGS | 0.000 | 0.000 | 0000 | 861 |
### Table 12. Catalog of thermochemical measurements at 298.15 K: heat capacity data

<table>
<thead>
<tr>
<th>No.</th>
<th>Reaction</th>
<th>Property Measured</th>
<th>Observed</th>
<th>Unc.</th>
<th>Residual Obs.-calc.</th>
<th>Reference</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>C(<em>6)H(</em>{12})O(_5)(\text{ao}) + H(_2)O(l) = C(<em>6)H(</em>{12})O(_5)(\text{ao}) + HPO(_4)^{2-}(\text{ao})</td>
<td>(\Delta C_p)</td>
<td>-48.</td>
<td>20.</td>
<td>-6.681</td>
<td>88TEW/STE</td>
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<td></td>
<td>(\Delta C_p) of hydrolysis of glucose-6P</td>
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<tr>
<td>2</td>
<td>C(<em>6)H(</em>{12})O(_5)(\text{ao}) + H(_2)O(l) = C(<em>6)H(</em>{12})O(_5)(\text{ao2}) + HP0(_4)^{2-}(\text{ao})</td>
<td>(\Delta C_p)</td>
<td>-46.</td>
<td>10.</td>
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<td>(\Delta C_p) of hydrolysis of mannose-6P</td>
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<td>3</td>
<td>C(<em>6)H(</em>{12})O(_5)(\text{ao}) + H(_2)O(l) = C(<em>6)H(</em>{12})O(_5)(\text{ao3}) + HP0(_4)^{2-}(\text{ao})</td>
<td>(\Delta C_p)</td>
<td>-28.</td>
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<td>21.299</td>
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<td>(\Delta C_p) of hydrolysis of fructose-6P</td>
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<td>4</td>
<td>C(<em>6)H(</em>{12})O(_5)(\text{ao}) + H(_2)O(l) = C(<em>6)H(</em>{12})O(_5)(\text{ao}) + HPO(_4)^{2-}(\text{ao})</td>
<td>(\Delta C_p)</td>
<td>-43.</td>
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<td>(\Delta C_p) of hydrolysis of ribose-5P</td>
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<td>5</td>
<td>C(<em>6)H(</em>{12})O(_5)(\text{ao2}) + H(_2)O(l) = C(<em>6)H(</em>{12})O(_5)(\text{ao2}) + HPC(_4)^{2-}(\text{ao})</td>
<td>(\Delta C_p)</td>
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<td>(\Delta C_p) of hydrolysis of ribulose-5P</td>
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<td>6</td>
<td>C(<em>6)H(</em>{12})O(_5)(\text{ao}) = C(<em>6)H(</em>{12})O(_5)(\text{ao4})</td>
<td>(\Delta C_p)</td>
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<td>(\Delta C_p) of isomerization of glucose-6P to fructose-6P</td>
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<td>C(<em>6)H(</em>{12})O(_5)(\text{ao3}) = C(<em>6)H(</em>{12})O(_5)(\text{ao4})</td>
<td>(\Delta C_p)</td>
<td>38.</td>
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<td>(\Delta C_p) of isomerization of mannose-6P to fructose-6P</td>
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<td>8</td>
<td>C(<em>6)H(</em>{12})O(_5)(\text{ao}) = C(<em>6)H(</em>{12})O(_5)(\text{ao3})</td>
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<td>C(<em>6)H(</em>{12})O(_5)(\text{ao}) = C(<em>6)H(</em>{12})O(_5)(\text{ao4})</td>
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<td>C(<em>6)H(</em>{12})O(_5)(\text{ao}) = C(<em>6)H(</em>{12})O(_5)(\text{ao7})</td>
<td>(\Delta C_p)</td>
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<td>90.</td>
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<td>( \mathrm{C}<em>{6}\mathrm{H}</em>{12}\mathrm{N}<em>{2}\mathrm{O}</em>{3}\mathrm{P}<em>{2}^{-}(\text{ao}) + \mathrm{H}<em>2\text{O}(\text{l}) = \mathrm{C}</em>{6}\mathrm{H}</em>{12}\mathrm{N}<em>{2}\mathrm{O}</em>{3}\mathrm{P}_{2}^{-}(\text{ao}) + \mathrm{HPO}_4^{2-}(\text{ao}) + \mathrm{H}^+(\text{ao}) )</td>
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<td>( \Delta C_p ) of hydrolysis of ATP</td>
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<td>( \mathrm{C}<em>{6}\mathrm{H}</em>{12}\mathrm{O}<em>{6}(\text{ao}) + \mathrm{C}</em>{6}\mathrm{H}<em>{12}\mathrm{N}</em>{2}\mathrm{O}<em>{3}\mathrm{P}</em>{2}^{2-}(\text{ao}) = \mathrm{C}<em>{6}\mathrm{H}</em>{12}\mathrm{O}<em>{6}(\text{ao})^3^- + \mathrm{C}</em>{6}\mathrm{H}<em>{12}\mathrm{N}</em>{2}\mathrm{O}<em>{3}\mathrm{P}</em>{2}^{2-}(\text{ao})^2 + \mathrm{H}^+(\text{ao}) )</td>
<td>( \Delta C_p )</td>
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<td>( \mathrm{C}<em>{6}\mathrm{H}</em>{12}\mathrm{O}<em>{6}(\text{ao2}) + \mathrm{C}</em>{6}\mathrm{H}<em>{12}\mathrm{N}</em>{2}\mathrm{O}<em>{3}\mathrm{P}</em>{2}^{-}(\text{ao}) = \mathrm{C}<em>{6}\mathrm{H}</em>{12}\mathrm{O}<em>{6}(\text{ao})^3^- + \mathrm{C}</em>{6}\mathrm{H}<em>{12}\mathrm{N}</em>{2}\mathrm{O}<em>{3}\mathrm{P}</em>{2}^{-}(\text{ao})^2 + \mathrm{H}^+(\text{ao}) )</td>
<td>( \Delta C_p )</td>
<td>10.</td>
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<td>233.089</td>
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<td>( \Delta C_p ) of phosphorylation (ATP) of mannose</td>
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<td>14</td>
<td>( \mathrm{C}<em>{6}\mathrm{H}</em>{12}\mathrm{O}<em>{6}(\text{ao3}) + \mathrm{C}</em>{6}\mathrm{H}<em>{12}\mathrm{N}</em>{2}\mathrm{O}<em>{3}\mathrm{P}</em>{2}^{-}(\text{ao}) = \mathrm{C}<em>{6}\mathrm{H}</em>{12}\mathrm{O}<em>{6}(\text{ao})^3^- + \mathrm{C}</em>{6}\mathrm{H}<em>{12}\mathrm{N}</em>{2}\mathrm{O}<em>{3}\mathrm{P}</em>{2}^{-}(\text{ao})^2 + \mathrm{H}^+(\text{ao}) )</td>
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<td>( \Delta C_p ) of phosphorylation (ATP) of fructose</td>
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<td>( \mathrm{HPO}_4^{2-}(\text{ao}) )</td>
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<td>[11KAW/KUS]</td>
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<td>C₆H₁₂O₆(cr) = C₆H₁₂O₆(aq)</td>
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<td>C₆H₁₂O₆(cr) = C₆H₁₂O₆(aq)</td>
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Table 12. Catalog of thermochemical measurements at 298.15 K: heat capacity data — Continued.
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<td>$C_6H_{12}O_6$(cr4) = $C_6H_{12}O_6$(ao3)</td>
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<td>$C_6H_{12}O_6P^-$ (ao2) = $C_6H_{12}O_6P^2$ (ao2) + $\mathcal{H}^+$ (ao)</td>
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<td>C₃H₇O₇(ao8) = C₃H₇O₇¹⁺(ao8) + H⁺(ao) 1st ionization of lyxose Based on enthalpies at two temperatures</td>
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<td>68</td>
<td>C₃H₇O₇(ao) = C₃H₇O₇¹⁺(ao) + H⁺(ao) 1st ionization of glucose Based on enthalpies at two temperatures</td>
<td>ΔC_p</td>
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<td>40</td>
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<td>70CHR/RYT</td>
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<td>C₃H₇O₇(ao2) = C₃H₇O₇¹⁺(ao2) + H⁺(ao) 1st ionization of mannose Based on enthalpies at three temperatures</td>
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<td>C₃H₇O₇(ao3) = C₃H₇O₇¹⁺(ao3) + H⁺(ao) 1st ionization of fructose Based on enthalpies at two temperatures</td>
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<td>C₃H₇O₇(ao4) = C₃H₇O₇¹⁺(ao4) + H⁺(ao) 1st ionization of galactose Based on enthalpies at two temperatures</td>
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<td><strong>Compound</strong></td>
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<tr>
<td>C$<em>6$H$</em>{12}$O$_6$P$_5$$^-$(ao6)</td>
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<td>galactose 1-phosphate$^-$(ao)</td>
<td>283, 284, 287, 350, 350, 350, 289</td>
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Table 13. Index to the compounds and their reactions in reference to Tables 11 and 15 — Continued

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<td>C₆H₁₂O₇P⁻(ao4)</td>
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<tr>
<td>C₆H₁₂O₇P(ao)</td>
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<td>C₆H₁₂O₇P(ao2)</td>
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<tr>
<td>C₆H₁₂O₇P(ao6)</td>
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<tr>
<td>NiC₃H₆O₇P(ao)</td>
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<td>Ni-ribose 5-phosphate(ao)</td>
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<tr>
<td>MgC₃H₆O₇P(ao)</td>
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<td>Mg-fructose 6-phosphate(ao)</td>
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<td>CaC₃H₆O₇P(ao2)</td>
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Table 14. Index to the compounds and their reactions in reference to Table 12 and the heat capacity data in Table 15

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<td>C₅H₁₀O₇(C)</td>
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<td>C₅H₁₀O₇(GI)</td>
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<td>C₅H₁₀O₇ (ao)</td>
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Table 15. Calculated values of thermochemical properties at 298.15 K

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<tr>
<th>Compound</th>
<th>molar mass g mol⁻¹</th>
<th>ΔH° kJ mol⁻¹</th>
<th>ΔG° kJ mol⁻¹</th>
<th>S° J mol⁻¹ K⁻¹</th>
<th>C°</th>
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<td>C₄H₈O₆(α-1)</td>
<td>148.1166</td>
<td>-900.455±7.4</td>
<td>-587.766±6.0</td>
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<td>xylose(αo)</td>
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<tr>
<td>C₆H₁₂O₆(α-5)</td>
<td>148.1166</td>
<td>-997.903±0.27</td>
<td>-669.666±6.0</td>
<td>93.304±20.0</td>
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<td>arabinose(α-5)</td>
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<td>C₆H₁₂O₆(cr)</td>
<td>149.1240</td>
<td>-1008.040±1.6</td>
<td>-681.085±2.3</td>
<td>97.604±9.3</td>
<td>176.0±45.0</td>
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<tr>
<td>ribose(cr)</td>
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<tr>
<td>C₆H₁₂O₆(cr2)</td>
<td>149.1240</td>
<td>-1003.787±0.39</td>
<td>-671.786±6.0</td>
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<td>165.0±45.0</td>
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<td>β-arabinose(cr)</td>
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<td>C₆H₁₂O₆(cr3)</td>
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<td>C₆H₁₂O₆(cr4)</td>
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<td>-730.086±6.0</td>
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<td>C₆H₁₂O₆(r)</td>
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<td>C₆H₁₂O₆(aa3)</td>
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<td>-1045.740±1.5</td>
<td>-750.485±2.2</td>
<td>203.87±8.9</td>
<td>279.0±20.0</td>
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<td>C₆H₁₂O₆(α-2)</td>
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<td>-594.236±2.4</td>
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<tr>
<td>C₆H₁₂O₆(α-4)</td>
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<td>-679.452±2.2</td>
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### Table 15. Calculated values of thermochemical properties at 298.15 K — Continued

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<th>Compound</th>
<th>molar mass g mol⁻¹</th>
<th>$\Delta H^\circ$</th>
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<td>$\text{C}_4\text{H}_6\text{O}_5$ (cr)</td>
<td>180.1577</td>
<td>-1273.040±0.87</td>
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<td>210.998±10.0</td>
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<td>$\beta$-glucose (cr)</td>
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<td>-906.333±0.17</td>
<td>203.400±0.43</td>
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<td>$\beta$-fructose (cr)</td>
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<td>$\text{C}_4\text{H}_6\text{O}_5$ (cr7)</td>
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<td>$\text{C}_6\text{H}_12\text{O}_6$ (cr)</td>
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<td>128.130±6.9</td>
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<td>glucose 6-phosphate ³⁻ (ao)</td>
<td>258.1228</td>
<td>-2277.436±1.2</td>
<td>-1763.942±2.0</td>
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Table 15. Calculated values of thermochemical properties at 298.15 K — Continued

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<th>Compound</th>
<th>molar mass g mol(^{-1})</th>
<th>(\Delta H^*) kJ mol(^{-1})</th>
<th>(\Delta G^*) kJ mol(^{-1})</th>
<th>(S^*) J mol(^{-1}) K(^{-1})</th>
<th>(C_v^*) J mol(^{-1}) K(^{-1})</th>
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### Auxiliary Data

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<td>${\Delta H'(pentose(ao)) - \Delta H'(pentose(cr))}$</td>
<td>($-13$ to $+14$) kJ mol$^{-1}$</td>
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<tr>
<td>${\Delta H'(hexose(ao)) - \Delta H'(hexose(cr))}$</td>
<td>(4.6 to 17.1) kJ mol$^{-1}$</td>
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<tr>
<td>${\Delta H'(sugar(ao)) - \Delta H'(sugar-phosphate(ao))}$</td>
<td>(1001 to 1015) kJ mol$^{-1}$</td>
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<tr>
<td>$\Delta G'(pentose(cr))$</td>
<td>($-730$ to $-745$) kJ mol$^{-1}$</td>
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<tr>
<td>$\Delta G'(hexose(cr))$</td>
<td>($-902$ to $-909$) kJ mol$^{-1}$</td>
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<tr>
<td>$\Delta G'(pentose(ao))$</td>
<td>($-739$ to $-731$) kJ mol$^{-1}$</td>
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<tr>
<td>$\Delta G'(hexose(ao))$</td>
<td>($-909$ to $-916$) kJ mol$^{-1}$</td>
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<tr>
<td>${\Delta G'(pentose(ao)) - \Delta G'(pentose(cr))}$</td>
<td>($-4.5$ to $-8.7$) kJ mol$^{-1}$</td>
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<tr>
<td>${\Delta G'(hexose(ao)) - \Delta G'(hexose(cr))}$</td>
<td>($-2.6$ to $-9.9$) kJ mol$^{-1}$</td>
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<tr>
<td>$\Delta G'(sugar(ao)) - \Delta G'(sugar-phosphate(ao))$</td>
<td>(630 to 820) kJ mol$^{-1}$</td>
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</tbody>
</table>
11. Reference Codes and References in the Tables

00LOB/EKE Lobry de Bruyn, C. A.; van Ekenstein, W. A.; Rec. Trav. Chim.; 19, 7 (1900)
00OSA Osaka, Y.; Z. Phys. Chem. (Leipzig); 35, 661 (1900)
01MAD Madsen, T.; Z. Phys. Chem. (Leipzig); 36, 290 (1901)
01MAG Magie, W. F.; Phys. Rev.; 13, 91 (1901)
13MIC/RON Michaelis, L.; Rona, P.; Biochem. Z.; 49, 284 (1913)
17DEH Dehn, W. M.; J. Am. Chem. Soc.; 39, 1399 (1917)
18PRA Pratt, F. R.; J. Franklin Inst.; 185, 663 (1918)
23GIL Gillis, J.; Rec. Trav. Chim.; 42, 1077 (1923)
25RIB/ESP Riber, C. N.; Esp, V.; Ber.; 58, 737 (1925)
26MEY/LOH Meyerhof, O.; Lohmann, K.; Naturwiss.; 14, 1277 (1926)
26RIB/MIN Riber, C. N.; Minsaas, J.; Ber.; 59, 2266 (1926)
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29HIR/SCH Hirsch, P.; Schlags, R.; Z. Phys. Chem. (Leipzig); 141, 387 (1929)
31MAR Marwick, T. C.; Proc. Roy. Soc. A; 131, 621 (1931)
34PAR/THO Parks, G. S.; Thomas, S. B.; J. Am. Chem. Soc.; 56, 1423 (1934)
36BEN/KRA Bennnewitz, K.; Kratz, L.; Physik. Z.; 37, 496 (1936)
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40GRE/RED Greenwald, I.; Redish, J.; Kibbrick, A. C.; J. Biol. Chem.; 135, 65 (1940)
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43KOS Kosterlitz, H. W.; Biochem J.; 37, 321 (1943)
49MEY/GRE Meyerhof, O.; Green, H.; J. Biol. Chem.; 178, 655 (1949)
50LAN/MAR Lange, E.; Markgraf, H. G.; Z. Elektrochem.; 54, 73 (1950)
50SLE Stein, M. W.; J. Biol. Chem.; 186, 753 (1950)
52LEL/CAR Leloir, L. F.; Cardini, C. E.; Cabib, E.; Annals Assoc. Quim. Arg.; 40, 228 (1952)
52THA Thamsen, J.; Acta Chem. Scand.; 6, 270 (1952)
52TRE/MAN Trevleyan, W. E.; Mann, P. F. E.; Harrison, J. S.; Arch. Biochem. Biophys.; 39, 419 (1952)
52TRE/MAN2 Trevleyan, W. E.; Mann, P. F. E.; Harrison, J. S.; Arch. Biochem. Biophys.; 39, 440 (1952)
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\textbf{CLA/CUS} Clarke, H. B.; Cusworth, D. C.; Datta, S. P.; Biochem. J.; 56, 14 (1954)
\textbf{CLA/CUS2} Clarke, H. B.; Cusworth, D. C.; Datta, S. P.; Biochem. J.; 58, 146 (1954)
\textbf{GIN} Ginodman, L. M.; Biochimia (Moscow); 19, 666 (1954)
\textbf{AXE} Axelrod, B.; Methods Enzymol.; 1, 363 (1955)
\textbf{DIC/WIL} Dickens, F.; Williamson, D. H.; Nature; 176, 400 (1955)
\textbf{VAR/WEB} Varner, J. E.; Webster, G. C.; Plant Phys.; 30, 393 (1953)
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\textbf{STU/HOR} Stumpf, P. K.; Horecker, B. L.; J. Biol. Chem.; 218, 753 (1956)
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\textbf{NOL/BRU} Noltmann, E.; Brunf, F. H.; Biochem. Z.; 330, 514 (1958)
\textbf{TAP/SRE} Tabachnick, M.; Serre, P. A.; Cooper, J.; Racker, E.; Arch. Biochem. Biophys.; 74, 315 (1958)
\textbf{WOO} Woolfson, M. W.; Acta Cryst.; 11, 393 (1958)
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12. Glossary of Symbols and Terminology

Roman
- **c**: concentration/mol L$^{-1}$; or parameter in expression for the excess heat capacity; or specific heat capacity/J kg$^{-1}$
- **e**: parameter in expression for the excess expansivity
- **g**: parameter in expression for the excess Gibbs energy
- **h**: parameter in expression for the excess enthalpy
- **k**: parameter in expression for the excess compressibility
- **m**: molality/ mol kg$^{-1}$
- **n**: amount of substance
- **p**: pressure/ Pa
- **u**: speed of sound/ m s$^{-1}$
- **v**: parameter in expression for the excess volume
- **x**: mole fraction

Greek
- **$\alpha$**: cubic expansion coefficient: $V^{-1}(\partial V/\partial T)_p$
- **$\gamma$**: activity coefficient
- **$\eta$**: viscosity
- **$\kappa_S$**: cubic isentropic compressibility coefficient
- **$\kappa_T$**: cubic isothermal compressibility coefficient
- **$\rho$**: (mass) density/ kg m$^{-3}$
- **$\phi$**: osmotic coefficient
- **$\Delta$**: change in a property

Superscripts
- **s**: standard state quantity
- *****: the property of the pure substance
- **∞**: the limit of a property as the concentration of solute approaches zero
- **ex**: excess
- **id**: ideal

Subscripts
- **f**: formation property
- **1, 2**: designate solvent and solute, respectively; the subscript 2 is frequently omitted for the solute
- **1, 2,...**: subscripts for virial parameters
- **φ**: apparent molar quantity

Physical states
- **am**: amorphous solid
- **ao**: aqueous, standard state of the indicated species
- **aq**: aqueous solution, concentration not specified
- **cr**: crystalline solid
- **g**: gaseous
- **l**: liquid
- **v**: vitreous (glassy) liquid

*When more than one meaning is attached to a given symbol, the context will serve to clarify the meaning of the symbol at that point in the text.*