

NATIONAL BUREAU OF STANDARDS REPORT

9501

TENTH PRELIMINARY REPORT ON A SURVEY OF THERMODYNAMIC PROPERTIES OF THE COMPOUNDS OF THE ELEMENTS CHNOPS

Progress Report for the Period 1 October to 31 December 1966

to

National Aeronautics and Space Administration

1 March 1967



U. S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

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George T. Furukawa, Martin L. Reilly
Gerald D. Mitchell, George T. Armstrong
Heat Division, Institute for Basic Standards

Progress Report for the Period 1 October to 31 December 1966

to

National Aeronautics and Space Administration

Contract No. R-138, Amendment 2.

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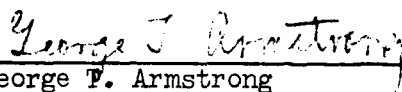
TABLE OF CONTENTS

	<u>Page</u>
Foreword	i
Section I. Analysis of Heat-Capacity and Vapor-Pressure Data	
George T. Furukawa and Martin L. Reilly . .	1
Section II. Gibbs Energies, Entropies and Enthalpies of Solution, Dilution, and Formation of Selected Ubiquitous Compounds	
Gerald D. Mitchell and George T. Armstrong .	2

FOREWORD

A study at the National Bureau of Standards (NBS), of which this is the tenth progress report, has been undertaken to meet the need of the National Aeronautics and Space Administration (NASA) for thermodynamic information on biologically related materials important to the space program for several reasons. Among these reasons are the necessity of inferring the maximum amount of useful chemistry of incompletely accessible environments, for which only limited information is available, the possibility of the occurrence of organic compounds naturally synthesized under primitive conditions, and the possibility of theoretically recovering part of the prebiological history of the earth.

This program is being carried out under the technical supervision of Dr. George Jacobs of NASA, and with the consultation of Dr. Harold Morowitz of the Yale University, Department of Molecular Biology and Biophysics, and Dr. C. W. Beckett of the Heat Division, Institute for Basic Standards (NBS). The contract (Contract No. R-138) was initiated 1 May 1964 and extended 29 April 1965. The program has been extended by Amendments 1 and 2. This report covers the first quarter of the work being carried out under Amendment 2.



George F. Armstrong
Supervisory Chemist
Project Leader

Section I

Analysis of Heat-Capacity and Vapor-Pressure Data

George T. Furukawa and Martin L. Reilly

The analysis of heat-capacity data has been directed largely on the higher molecular weight C-H compounds. Intensive examination of the data showed inconsistencies in the published analyses of the observations in the "premelting" region for some of the substances. A new computer method was developed to perform an improved analysis of the data in this temperature range.

The compilation of vapor-pressure data is new to the group. There was, therefore, no immediate source of vapor-pressure data to carry out the analysis. An effort was started to compile vapor-pressure data on the same relatively high molecular weight C-H compounds for which the heat-capacity data were available. The existing compilations, such as those by Timmermans, Stull, etc., were consulted. A computer code for analyzing the vapor-pressure data is being developed.

The following is the list of C-H compounds on which the analysis of heat-capacity data is in various stages of completion and for which the vapor-pressure data are being compiled:

- A. normal paraffins: C_9 , C_{10} , C_{11} , C_{12} , C_{13} , C_{14} , C_{15} , C_{16} ,
 C_{32} , and C_{36} .
- B. aromatic hydrocarbons: benzene, naphthalene, anthracene,
phenanthrene, pyrene, 1-methylnaphthalene,
and 2-methylnaphthalene.
- C. others: tetralin, cis-decalin, trans-decalin, and adamantane.

The relatively old heat-capacity data on alloxan, allantoin, uric acid, xanthine, guanine, hypoxanthine, and lactic acid for which measurements extend down only to about 80°K have been re-examined to obtain a better extrapolation to 0°K. Further efforts are still needed at this time to reduce the uncertainty of the extrapolation.

Section II

Gibbs Energies, Entropies and Enthalpies of Solution, Dilution, and Formation of Selected Ubiquitous Compounds

Gerald D. Mitchell and George T. Armstrong

A selected list of amino acids, purine and pyrimidine bases, sugars, fatty acids, glycerol, was the basis of a search for additional thermodynamic data beyond that published in our previous reports. The heat, entropy, and Gibbs energy of formation in the free state, the enthalpies, entropies and Gibbs energies of solution, the enthalpies of dilution and the Gibbs energy of formation of the aqueous state were found for many but not all of these substances. A list of the compounds with a description of the data selected for each follows, including values from our previous work when they existed. The discussion gives a reference to the source of the data in the following list of references. Numerous gaps exist in the data.

Table 1.

Selected Thermodynamic Data

L-Alanine

$$\underline{\Delta G_{298}^{\circ}, \Delta S_{298}^{\circ}}$$

Gibbs energy and entropy of formation are given by Domalski [6]* from data given in previous reports. $\Delta G_{298}^{\circ} = -87.94 \text{ kcal mol}^{-1}$; $\Delta S_{298}^{\circ} = -154.34 \text{ cal(deg mol)}^{-1}$.

$$\underline{\Delta H_{298}^{\circ}}$$

The heat of formation reported in [6] was taken from Table 1, NBS Report 8641, p. 12 [7].

$$\underline{\Delta H_{298}(\text{solution})}$$

The heat of solution as determined calorimetrically by Zittle is $\Delta H_{298} = 2140 \pm 30 \text{ cal mol}^{-1}$ [12].

$$\underline{\Delta H_{298}(\text{dilution})}$$

The heat of dilution as determined directly by Zittle is $\Delta H_{298} = 210 \text{ cal mol}^{-1}$ [12].

$$\underline{\Delta G_{298}(\text{in solution})}$$

Krebs and Kornberg [5] list Burton and Krebs [14] value for ΔG_{298} of formation in solution, $-88.75 \text{ kcal mol}^{-1}$.

$$\underline{\Delta G_{298}(\text{of solution})}$$

The Gibbs energy of solution of L-alanine is given in [13] by Greenstein. $\Delta G_s = -350 \text{ cal mol}^{-1}$.

$$\underline{\Delta S_{298}(\text{of solution})}$$

Calculated from existing data, ΔG_s [13] and ΔH_s [9], $\Delta S_{298}^{\circ} = 8.0161 \text{ cal(deg mol)}^{-1}$.

* Figures in brackets indicate literature references listed at end of this chapter.

l-Arginine

$$\underline{\Delta H_{298}^{\circ}}$$

Domalski and Halow [7] list Huffman, Fox, and Ellis [15] value of the heat of formation $\Delta H_{298}^{\circ} = -148.66 \text{ kcal mol}^{-1}$.

$$\underline{\Delta G_{298}^{\circ}}$$

Gibbs energy of formation of pure substance is given by Krebs and Kornberg [5], taken from Huffman and Ellis [16], $\Delta G_{298}^{\circ} = 57.44 \text{ kcal mol}^{-1}$.

$$\underline{\Delta S_{298}^{\circ}}$$

Data calculated from ΔH_{298}° and ΔG_{298}° given in [7] and [5] respectively, $\Delta S_{298}^{\circ} = -305.95 \text{ cal(deg mol)}^{-1}$.

$$\underline{\Delta H_{298}(\text{of solution})}$$

The heat of solution of l-arginine, $\Delta H_{298} = 1500 \text{ cal mol}^{-1}$, is given by Zittle and Schmidt [12].

l-Aspartic Acid

$$\underline{\Delta H_{298}^{\circ}}, \underline{\Delta S_{298}^{\circ}}, \underline{\Delta G_{298}^{\circ}}$$

Data taken from [6] as given by Domalski, $\Delta H_{298}^{\circ} = -232.47 \text{ kcal mol}^{-1}$, $\Delta S_{298}^{\circ} = -194.94 \text{ cal(deg mol)}^{-1}$, $\Delta G_{298}^{\circ} = -174.35 \text{ kcal mol}^{-1}$.

$$\underline{\Delta H_{298}(\text{of solution})}$$

Data obtained by direct measurement is given by Zittle and Schmidt [12]. $\Delta H_{298} = 6000 \text{ cal mol}^{-1}$.

$$\underline{\Delta G_{298}(\text{in solution})}$$

Krebs and Kornberg [5] report the value of Burton and Krebs [14]. $\Delta G_{f298} = 172.31 \text{ kcal mol}^{-1}$.

$$\underline{\Delta G_{298}(\text{of solution})}$$

Greenstein [13] reports ΔG_s to be $+2550 \text{ cal mol}^{-1}$.

$$\underline{\Delta S_{298}(\text{solution})}$$

Calculated from ΔH_s and ΔG_s given in [12] and [13], respectively. $\Delta S_{298} = 11.5714 \text{ cal(deg mol)}^{-1}$.

L-Asparagine·H₂O

$$\underline{\Delta H_{298}^{\circ}, \Delta S_{298}^{\circ}, \Delta G_{298}^{\circ}}$$

Heat, Gibbs energy, and entropy of formation. Data from Domalski [6]. $\Delta H_{298}^{\circ} = -259.52 \text{ kcal mol}^{-1}$, $\Delta S_{298}^{\circ} = -255.19 \text{ cal(deg mol)}^{-1}$, $\Delta G_{298}^{\circ} = -183.44 \text{ kcal mol}^{-1}$.

$$\underline{\Delta H_{298}(\text{of solution})}$$

The experimental value as determined by Dalton and Schmidt [8] is $\Delta H_{298} = 8000 \text{ cal mol}^{-1}$.

$$\underline{\Delta G_{298}(\text{in solution})}$$

Krebs and Kornberg [5] report Barsook and Huffman [18] value, $\Delta G_{298} = -125.86 \text{ kcal mol}^{-1}$.

$$\underline{\Delta G_{298}(\text{of solution})}$$

Greenstein [13] reports the value of $+950 \text{ cal mol}^{-1}$ for the Gibbs energy of solution.

$$\underline{\Delta S_{298}(\text{of solution})}$$

We calculated $\Delta S = 23.6458 \text{ cal(deg mol)}^{-1}$ from data in [8] and [13], ΔH , ΔG respectively.

Cysteine

$$\underline{\Delta G_{298}^{\circ} \text{ (pure compound)}}$$

Krebs and Kornberg [5] report values calculated from Barsook, Ellis and Huffman [17], $\Delta G_{298}^{\circ} = -163.55 \text{ kcal mol}^{-1}$.

$$\underline{\Delta G_{298}^{\circ}(\text{in solution})}$$

$\Delta G_{298}^{\circ} = -159.00$ listed by Krebs and Kornberg [5], calculated from Barsook, Ellis and Huffman [17].

Glutamic Acid

$$\underline{\Delta H_{298}^{\circ}}, \underline{\Delta S_{298}^{\circ}}, \underline{\Delta G_{298}^{\circ}}$$

Data reported by Domalski [6]. $\Delta H_{298}^{\circ} = -240.05 \text{ kcal mol}^{-1}$;
 $\Delta S_{298}^{\circ} = -223.19 \text{ cal(deg mol)}^{-1}$; $\Delta G_{298}^{\circ} = -173.51 \text{ kcal mol}^{-1}$.

$$\underline{\Delta H_{298}(\text{solution})}$$

Zittle and Schmidt [12] report a value for the heat of solution,
 $\Delta H_s = 6530 \text{ cal mol}^{-1}$.

$$\underline{\Delta G_{298}(\text{in solution})}$$

Krebs and Kornberg [5] report Borsook and Huffman's [18] data for
the Gibbs energy of formation in aq. solution, $\Delta G_{298} = -171.75 \text{ kcal mol}^{-1}$.

$$\underline{\Delta G_{298}(\text{of solution})}$$

The value for the Gibbs energy of solution is given in [13] by
Greenstein. $\Delta G_s = 2300 \text{ kcal mol}^{-1}$.

$$\underline{\Delta S_{298}^{\circ}(\text{of solution})}$$

Calculated from data in [12] and [13], $\Delta S_s^{\circ} = 14.1875 \text{ cal(deg mol)}^{-1}$.

Glutamine

$$\underline{\Delta H_{298}^{\circ}}, \underline{\Delta S_{298}^{\circ}}, \underline{\Delta G_{298}^{\circ}}$$

Data given by Domalski [6] is taken from previous reports.
 $\Delta H_{298}^{\circ} = -197.8 \text{ kcal mol}^{-1}$, $\Delta S_{298}^{\circ} = -235.53 \text{ cal(deg mol)}^{-1}$,
 $\Delta G_{298}^{\circ} = -127.60 \text{ kcal mol}^{-1}$.

Glycine

$$\underline{\Delta H_{298}^{\circ}}, \underline{\Delta S_{298}^{\circ}}, \underline{\Delta G_{298}^{\circ}}$$

The value given by Domalski [6] is taken from previous reports.
 $\Delta H = -126.22 \text{ kcal mol}^{-1}$, $\Delta S_{298}^{\circ} = -127.88 \text{ cal(deg mol)}^{-1}$,
 $\Delta G_{298}^{\circ} = -88.09 \text{ kcal mol}^{-1}$.

$$\underline{\Delta H_{298}(\text{of solution})}$$

Zittle and Schmidt [12] report a value of $3750 \text{ cal mol}^{-1}$.

ΔH_{298} (of dilution)

Zittle and Schmidt [12] give an experimental value of 225 cal mol^{-1} .

ΔG_{298} (in solution)

Reported by Krebs and Kornberg [5], taken from Rossini et al. [19],
 $\Delta G_{298} = -89.26 \text{ kcal mol}^{-1}$.

ΔG_{298} (of solution)

Greenstein and Winitz [13] give the Gibbs energy of solution as
 $-650 \text{ cal mol}^{-1}$.

ΔS_{298} (of solution)

Calculated from data given in [12,13], ΔH_{298} , ΔG_{298} of solution.
 $\Delta S_{298} = 14.7577 \text{ cal(deg mol)}^{-1}$.

L-Histidine

ΔH (of solution)

Zittle and Schmidt [12] give a value of $3300 \text{ cal mol}^{-1}$ for the
heat of solution.

ΔH_{298} (dilution)

Greenstein and Winitz [13] give -90 cal mol^{-1} as the heat of dilution.

L-Isoleucine

ΔH_{298}° , ΔG_{298}° , ΔS_{298}°

Domalski in [6] gives the values $\Delta H_{298}^{\circ} = -151.8 \text{ kcal mol}^{-1}$,
 $\Delta S_{298}^{\circ} = -233.33 \text{ cal(deg mol)}^{-1}$, $\Delta G_{298}^{\circ} = -82.2 \text{ kcal mol}^{-1}$.

ΔH° (of solution)

Dalton and Schmidt [8] report a calculated value of 843 cal mol^{-1} .

ΔG (of solution)

Greenstein and Winitz [13] report 700 cal mol^{-1} for the Gibbs
energy of solution.

ΔS (of solution)

Calculated from the data given in [8] and [13], ΔH_s and ΔG_s give
 $\Delta S_{298} = 0.4796 \text{ cal(deg mol)}^{-1}$.

Leucine

$$\Delta H_{298}^{\circ}, \Delta S_{298}^{\circ}, \Delta G_{298}^{\circ}$$

Domalski in reference [6] reports the values $\Delta H_{298}^{\circ} = -151.97$ kcal mol⁻¹, $\Delta S_{298}^{\circ} = -232.37$ cal(deg mol)⁻¹, and $\Delta G_{298}^{\circ} = -82.68$ kcal mol⁻¹.

$$\Delta G_{298}^{\circ}(\text{in solution})$$

Krebs and Kornberg [5] report Borsook and Huffman's [18] value adjusted (+0.03 K cal) for ΔG° of racemization. $\Delta G_{298}^{\circ} = -81.68$ kcal mol⁻¹.

$$\Delta G_{298}^{\circ}(\text{of solution})$$

Greenstein and Winitz [13] give the value of 950 cal mol⁻¹.

$$\Delta H_{298}^{\circ}(\text{of solution})$$

Dalton and Schmidt [9] report $\Delta H_{298} = 830$ cal mol⁻¹ corrected for activity of amino acid.

$$\Delta S_{298}^{\circ}(\text{of solution})$$

Calculated from ΔG_{298}° and ΔH_{298}° of solutions [13], [9].
 $\Delta S_{298}^{\circ} = -0.4025$ cal(deg mol)⁻¹.

Lysine

$$\Delta H_{298}^{\circ}$$

Domalski and Halow [7] report Ponomarev and Migarskaya [20] value $\Delta H_{298}^{\circ} = -162.2$ kcal mol⁻¹.

$$\Delta H_{298}^{\circ}(\text{of solution})$$

Zittle and Schmidt [12] give a value of 4000 ± 100 cal mol⁻¹.

$$\Delta H_{298}^{\circ}(\text{of dilution})$$

Greenstein and Winitz [13] give ΔH_{298}° of dilution to be 500 cal mol⁻¹.

l-Methionine

$$\underline{\Delta H_{298}^{\circ}}$$

Domalski and Halow [7] report Tsuzuki, Harper, and Hunt's [21] value $-180.4 \text{ kcal mol}^{-1}$.

$$\underline{\Delta S_{298}^{\circ}}$$

Hutchens, Cole, and Stout [10] report the entropy as calculated from the elements [19].

$$\underline{\Delta H_{298}(\text{of solution})}$$

Dalton and Schmidt [8] give an experimental value of $4100 \text{ cal mol}^{-1}$.

$$\underline{\Delta G_{298}(\text{of solution})}$$

Greenstein and Winitz [13] give 850 cal mol^{-1} for the Gibbs energy of solution.

$$\underline{\Delta S_{298}(\text{of solution})}$$

Calculated from the data in [8], [13], ΔG_{298} and ΔH_{298} of solution.
 $\Delta S_{298} = 10.5652 \text{ cal(deg mol)}^{-1}$.

l-Phenylalanine

$$\underline{\Delta H_{298}^{\circ}}, \underline{\Delta S_{298}^{\circ}}, \underline{\Delta G_{298}^{\circ}}$$

Domalski [6] reports the values $\Delta H_{298}^{\circ} = -111.9 \text{ kcal mol}^{-1}$,
 $\Delta S_{298}^{\circ} = -204.87 \text{ cal(deg mol)}^{-1}$ and $\Delta G_{298}^{\circ} = -50.6 \text{ kcal mol}^{-1}$.

$$\underline{\Delta H_{298}(\text{of solution})}$$

Dalton and Schmidt [9] give the corrected value of $2770 \text{ cal mol}^{-1}$ for the heat of solution.

$$\underline{\Delta G_{298}^{\circ}(\text{of solution})}$$

Greenstein and Winitz [13] report $1000 \text{ cal mol}^{-1}$ for the Gibbs energy of solution.

$$\underline{\Delta S_{298}^{\circ}(\text{of solution})}$$

Calculated from the data in [9,13], ΔH_{298} and ΔG_{298} of solution.
 $\Delta S_{298} = 5.9366 \text{ cal(deg mol)}^{-1}$.

Proline

$$\underline{\Delta H_{298}^{\circ}}, \underline{\Delta S_{298}^{\circ}}, \underline{\Delta G_{298}^{\circ}}$$

Domalski [6] reported the values $\Delta H_{298}^{\circ} = -125.7 \text{ kcal mol}^{-1}$,
 $\Delta S_{298}^{\circ} = -179.97 \text{ cal(deg mol)}^{-1}$, $\Delta G_{298}^{\circ} = -72.0 \text{ kcal mol}^{-1}$.

$$\underline{\Delta H_{298}(\text{of solution})}$$

Greenstein and Winitz [13] report 750 cal mol^{-1} for the heat of solution.

$$\underline{\Delta H_{298}(\text{dilution})}$$

Greenstein and Winitz [13] give an experimental value of $1050 \text{ cal mol}^{-1}$.

$$\underline{\Delta G_{298}(\text{of solution})}$$

Greenstein and Winitz [13] reports $-1450 \text{ cal mol}^{-1}$.

$$\underline{\Delta S_{298}(\text{of solution})}$$

Calculated from data in [13], ΔG_{298} and ΔH_{298} of solution.
 $\Delta S_{298} = 7.3788 \text{ cal(deg mol)}^{-1}$.

Serine

$$\underline{\Delta H_{298}^{\circ}}, \underline{\Delta S_{298}^{\circ}}, \underline{\Delta G_{298}^{\circ}}$$

Hutchins, Cole, and Stout [11] give experimental values of
 $\Delta H_{298}^{\circ} = -173.6 \text{ kcal mol}^{-1}$, $\Delta S_{298}^{\circ} = -174.06 \text{ cal(deg mol)}^{-1}$, and
 $\Delta G_{298}^{\circ} = -121.6 \text{ kcal mol}^{-1}$.

$$\underline{\Delta H_{298}}, \underline{\Delta G_{298}(\text{of solution})}$$

Greenstein and Winitz [13] report $\Delta H_{298} = 5180 \text{ cal mol}^{-1}$ and
 $\Delta G_{298} = 450 \text{ cal mol}^{-1}$ of solution.

$$\underline{\Delta S_{298}(\text{of solution})}$$

Calculated from data in [13], ΔS is $15.8645 \text{ cal(deg mol)}^{-1}$.

$$\underline{\Delta H_{298}(\text{dilution})}$$

Greenstein and Winitz's [13] experimental value is $-130 \text{ cal mol}^{-1}$.

Threonine

$$\Delta H_{298}^{\circ}$$

Domalski and Halow [7] report Tsuzuki, Harper and Hunter's [21] value for the heat of formation. $\Delta H_{298}^{\circ} = -181.4 \text{ kcal mol}^{-1}$.

$$\Delta G_{298}(\text{in solution})$$

Krebs and Kornberg [5] give Metzler, Langenecker, and Snell's [22] approximate value of $-123.0 \text{ kcal mol}^{-1}$.

Tryptophane

$$\Delta H_{298}^{\circ}, \Delta S_{298}^{\circ}, \Delta G_{298}^{\circ}$$

Domalski [6] gives the values $\Delta H_{298}^{\circ} = -99.8 \text{ kcal mol}^{-1}$, $\Delta S_{298}^{\circ} = -237.29 \text{ cal(deg mol)}^{-1}$, $\Delta G_{298}^{\circ} = -29.1 \text{ kcal mol}^{-1}$.

$$\Delta H_{298}(\text{of solution})$$

Dalton and Schmidt [8] give a calculated value of $1300 \text{ cal mol}^{-1}$ for the heat of solution.

$$\Delta G_{298}(\text{of solution})$$

Greenstein and Winitz [13] give a value of $1750 \text{ cal mol}^{-1}$ for the Gibbs energy of solution.

$$\Delta S_{298}(\text{of solution})$$

Calculated from the data in [8,13], ΔG_{298} , ΔH_{298} of solution. $\Delta S_{298} = -1.3081 \text{ cal(deg mol)}^{-1}$.

Tyrosine

$$\Delta H_{298}^{\circ}, \Delta S_{298}^{\circ}, \Delta G_{298}^{\circ}$$

Domalski [6] reports a value of $\Delta H_{298}^{\circ} = -163.4 \text{ kcal mol}^{-1}$, $\Delta S_{298}^{\circ} = -229.28 \text{ cal(deg mol)}^{-1}$, $\Delta G_{298}^{\circ} = -95.06 \text{ kcal mol}^{-1}$.

$$\Delta G_{298}(\text{in solution})$$

Krebs and Kornberg [5] report Huffman and Ellis' [16] value $-92.55 \text{ kcal mol}^{-1}$.

$$\Delta H_{298}(\text{of solution})$$

Dalton and Schmidt [9] give a corrected value of $5960 \text{ cal mol}^{-1}$ for the heat of solution.

ΔG_{290} (of solution)

Greenstein and Winitz [13] report $-3550 \text{ cal mol}^{-1}$ for the Gibbs energy of solution.

ΔS_{298} (of solution)

Calculated from data in [9,13], ΔH_{298} , ΔG_{298} of solution.
 $\Delta S_{298} = 31.8967 \text{ cal(deg mol)}^{-1}$.

Thymine

ΔH_{298}°

Domalski [6] gives a value of $-111.9 \text{ kcal mol}^{-1}$.

Valine

ΔH_{298}° , ΔS_{298}° , ΔG_{298}°

Domalski [6] reports the values $\Delta H_{298}^{\circ} = -1148.2 \text{ kcal mol}^{-1}$,
 $\Delta S_{298}^{\circ} = -207.67 \text{ cal(deg mol)}^{-1}$, $\Delta G_{298}^{\circ} = -286.3 \text{ kcal mol}^{-1}$.

ΔG_{298} , ΔH_{298} (of solution)

Greenstein and Winitz [13] give the values $\Delta G_{298} = 350 \text{ cal mol}^{-1}$,
 $\Delta H_{298} = 500 \text{ cal mol}^{-1}$.

ΔS_{298} (of solution)

Calculated from the data given by Greenstein and Winitz [13],
 ΔG_{298} and ΔH_{298} of solution. $\Delta S_{298} = 0.503 \text{ cal(deg mol)}^{-1}$.

D-Glucose

ΔH_{298}° , ΔS_{298}° , ΔG_{298}°

Burton and Krebs [3] report values of $\Delta H_{298}^{\circ} = -304.64 \text{ kcal mol}^{-1}$,
 $\Delta S_{298}^{\circ} = -291.7 \text{ cal(deg mol)}^{-1}$ and $\Delta G_{298}^{\circ} = -217.56 \text{ kcal mol}^{-1}$.

ΔG_{298} (in solution)

Burton and Krebs [3] report a value of $-219.38 \text{ kcal mol}^{-1}$.

ΔG_{298} (of solution)

Burton and Krebs [3] give the value of $-1820 \text{ cal mol}^{-1}$.

ΔH_{298} (of solution)

Taylor and Rowlinson [1] give a value of $2630 \pm 10 \text{ cal mol}^{-1}$.

ΔS_{298} (of solution)

The value $14.9254 \text{ cal}(\text{deg mol})^{-1}$ was calculated from data given by Burton and Krebs [26] and Taylor and Rowlinson [1].

ΔH_{298} (of dilution)

Lange and Markgraf [2] report an integral value of $28.55 \pm 0.16 \text{ cal mol}^{-1}$ for a solution that is 0.3479 M.

Ribose

ΔH_{298}°

Domalski and Halow [7] report a value of $-253.9 \text{ kcal mol}^{-1}$ for the heat of formation at 298.15°K .

Adenine

ΔH_{298}° , ΔS_{298}° , ΔG_{298}°

Stiehler and Huffman [4] report a calculated value of $-163.2 \text{ cal}(\text{deg mol})^{-1}$ for ΔS_{298}° , $-70.420 \text{ kcal mol}^{-1}$ for ΔG_{298}° and $-21.760 \text{ kcal mol}^{-1}$ for ΔH_{298}° .

Guanine

ΔH_{298}° , ΔS_{298}° , ΔG_{298}°

Stiehler and Huffman [4] give calculated values, $\Delta H_{298}^{\circ} = -45.090 \text{ kcal mol}^{-1}$, $\Delta S_{298}^{\circ} = -185.6 \text{ cal}(\text{deg mol})^{-1}$ and $\Delta G_{298}^{\circ} = 10.220 \text{ kcal mol}^{-1}$.

Butyric Acid

$$\underline{\Delta H_{298}^{\circ}}, \underline{\Delta S_{298}^{\circ}}, \underline{\Delta G_{298}^{\circ}}$$

Burton and Krebs [3] report the values $\Delta H_{298}^{\circ} = -128.09 \text{ kcal mol}^{-1}$, $\Delta S_{298}^{\circ} = -125.2 \text{ cal(deg mol)}^{-1}$, $\Delta G_{298}^{\circ} = -90.65 \text{ kcal mol}^{-1}$.

$$\underline{\Delta G_{298}(\text{in solution})}$$

Burton and Krebs [3] give $-91.2 \text{ kcal mol}^{-1}$ for ΔG_{298} in aq. solution.

$$\underline{\Delta G_{298}(\text{of solution})}$$

Burton and Krebs [3] report $-550 \text{ cal mol}^{-1}$ for the ΔG_{298} of solution.

Palmitic Acid

$$\underline{\Delta G_{298}^{\circ}}$$

Krebs and Kornberg [5] give Parks and Huffman's [3] value of $-25.7 \text{ kcal mol}^{-1}$ for the Gibbs energy of formation.

References to Section II

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