Physicochemical data in Landolt-Börnstein Online

Rainer Poerschke, Springer-Verlag, Berlin, Germany

0: Emphasis and method of the Landolt-Börnstein data collection

1. Historical and technical development from 1883-2002
2. Use of LB-Online, release 1.0, starting from the homepage **landolt-boernstein.com**
3. Examples in Physical Chemistry and Condensed Matter
4. Further development

0: **Emphasis and method of the Landolt-Börnstein data collection**

To create a **collection of reliable physical data and functional relationships in Science and Technology**

How to do this?

0. Landolt, Börnstein and their assistants did it themself for the Physical Chemistry and learned how it works

Already in the year 1882, Hans Landolt and Richard Börnstein, professors in chemistry and physics respectively founded the LB-collection.
A handwritten contract was closed in Berlin with Julius Springer, a bookseller and the founder of Springer Verlag(now operating internationally within the group BertelsmannSpringer within the Bertelsmann company).

1883 the first Landolt-Börnstein data handbook **Physikalisch Chemische Tabellen**

containing 280 pages was published.

A story of success: Thousands of copies selled, 5 further editions followed until 1980

The open/flexible New Series was founded by Karl Heinz Hellwege the language went from German to English

After approx. 120 years more than 1000 international experts and an editorial office of 5 scientists and 5 assistants are working for LB.

Until now **goal of Landolt-Börnstein:**

<u>High quality data recommended by international experts in the various fields</u>

I. Elementary Particles, Nuclei and Atoms

II. Molecules and Radicals

III. Condensed Matter-largest group with more than 150 (sub)volumes

IV. Physical Chemistry, I focus on this group today

Small groups:

V. Geophysics
VI. Astrophysics
VII. Biophysics
New VIII: Advanced Materials and Technologies

How to reach the goal today?

How to reach the Goal today:

1. Find experts for a distinct group of data and materials/substances/compounds

   And discuss a concept for their data collection with them.

2. Let the publisher make contracts with the experts and pay for their work.

   He has also the task of supporting the experts by an editorial office, which consits of scientists and assistants, who check and prepare the manuscripts for the production of print and electronic versions as well as special substance and property indexes. They use help of external companies for the drawing of figures(up to 5000 per year) and typesetting.

3. Collection of literature, selection of references, data, figures and metadata.

   The preparation of a manuscript takes 2-4 in some cases more years.

4. Check of the manuscript by the editor, acceptance or revision

5. Check of the manuscript by the editorial office, redrawing of figures*, text and tables reformatting if necessary.

   List of "stupid"questions(non-experts) to the editor and authors.

6. Finishing the Print-, CD-ROM- and Online-version after "Imprimatur" of the authors.

7. Decision publisher and editor-in chief together with volume editor,

"if and when supplementation or revised edition should be scheduled?"

Today new possibilities due to electronic publishing

"Online first for a more continous processing of the information"
Problem: "Who pays for that and how to pay for the work?"

History and development of the number of pages in the various editions.

How were the steps from the print version to LB-Online done?

I. Old volumes > 100.000 pages scanned with 300 dpi resolution
II. Transformation of page images into the Portable Data Format, pdf
III. Optical character recognition with Adobe Capture 2.0
IV. Special pdf-format keeps facsimile and has text in a second layer in the background

Millennium campaign offers free access in 2000 and 2001 to all volumes published until 1990 in a prerelease.

10.000 registered users, more than 2 Million pages were downloaded

Survey of the users: New design of Release 1.0

November 2001 all volumes were available in Release 1.0, 60 CD-ROMS published since 1998 were incorporated.

Examples from the group **Physical Chemistry of Landolt-Börnstein**:

Volume IV/8

Thermodynamic Properties of Liquid Pure Organic Compounds and their Mixtures

Here focus on the fundamental property: "**Density**"

1992 first meeting with Ken Marsh at the CODATA in Bejing
Soon starting cooperation of LB with TRC, now TRC/NIST, 15 subvolumes, i.e. 6000 pages, published.

Further Properties: "Enthalpies of Fusion and Transition", "Vapor Pressure of Chemicals", "Virial Coefficients"

The group headed by Michael Frenkel group members Quian Dong, Xinjian Yan, Roberto D. Chirico and Randolph C. Wilhoit, Ken Marsh and Ken Hall, former directors of TRC contributed as further authors, editors or co-editors.

For further details I refer to the two related presentations of Mrs. Quian Dong , NIST, Boulder, Co, USA, titles were:

1. Reliability of **uncertainty assignments** in generating recommended data
from a large set of experimental physiochemical data

2. **Knowledge management** in physiochemical property databases - knowledge recovery and retrieval of NIST/TRC source data system

   One sentence becomes special importance for Landolt-Börnstein, which is working with more than 1000 international experts as authors and editors:

In addition to the systematic and statistical uncertainties the **personal judgement and experience** of the experts is of eminent importance.

Certainly individual components are subjected to changes due to different experts and increasing knowledge.

Substance characterization by sum formulae, names(IUPAC, common, database) CAS-Reg.-No

Density values with uncertainties and literature citations

Temperature dependence

Fit of theoretical formulae, given in the introduction together with methods of measurement etc.

Deviation of the data points with their uncertainties from the best fit

Recommended values

Sometimes further references, the data of which were not presented.

Example 2:

Phase equilibria Phase Equilibria, Crystallographic and Thermodynamic Data of Binary Alloys

B. Predel,

With the Preliminary Co-operation of Kl. Schäfer †
Edited by O. Madelung

More than 500 journals

All phase diagrams in a unique style making comparisons and concentration determination easy

Combination of Phase diagrams, crystallographic and thermodynamic data yield knowledge

10 subvolumes published 1991-1998, first supplementation scheduled for 2003

Integration over all subvolumes electronically:

List of systems

Periodic table

How to find information in Landolt-Börnstein Online?

150.000 pages

1. Navigation by groups, sections, volumes, subvolumes, tables of contents/substance indexes

5. Navigation by overall indexes: A-Z

3. Substance Indexes Inorganic Organic -(sub)structure search in preparation

4. Fulltext Search in Landolt-Börnstein

4. Fulltext Search in Landolt-Börnstein

   in table of contents

   in documents(PDF)

   in titles of the documents

   for authors of documents

Preselection for groups

150.000 pages from 300 (sub)volumes, organized in 25.000 pdf documents

are accessible on LINK with navigation and preselected fulltext search

homepage: www.landolt-boernstein.com

Landolt-Börnstein is now online available in LINK!

Landolt-Börnstein is the unique and top-quality chemistry, physics and technology data collection bringing you the work of a thousand experts right to your screen. This handbook's data coverage starts with the scientific data described before 1883 - the year of the first handbook publication- up to 2002.

It is a systematic and comprehensive collection of critical assessed data from all fields of physics, physical chemistry, geophysics, astronomy, material technology and engineering and biophysics.

- each volume is a thoroughly supplemented and revised version of the predecessor
- continuously expanded to accommodate new data
- today the New Series comprises more than 270 volumes

Discover the benefits of the online version:

- full text PDFs available online
- excellent readability of table of contents
- clear and fast navigation in subvolumes with bookmarks in a hierarchical architecture or with frames and Java script table of contents (for the Millennium prerelease only).
- searchable via LB search

Topics covered by LB

Units and Fundamental Constants(of general interest, i.e. without a group)

- Elementary Particles, Nuclei and Atoms (Group I)
- Molecules and Radicals (Group II)
- Condensed Matter (Group III)
- Physical Chemistry (Group IV)
- Geophysics (Group V)

LB-Online – Navigation and Search

1. An easy-to-use and link-supported navigation takes you through the Landolt-Börnstein data collection step by step:

- LB Home Page
  - LB Groups
    - Volume within a Group
      - Subvolume
        - Table of Contents of Subvolume
          - FullText PDF-Files

Please note that the fulltext pdf-files are accessible to subscribers only, except those marked with the FREE online button, which are accessible free-of-charge.

Navigation within the Table of Contents of a subvolume is supported by bookmarks. A click on a bookmark takes you to the respective fulltext pdf-file which will then appear in the right frame.

For optimal navigation, we recommend installing Acrobat Reader (version 4.0) as a plug-in.

Please do not hesitate to inform us if any problems or questions arise whilst browsing through Landolt-Börnstein in LINK. We would like to hear about your ideas on how to improve our system. Please send your mail to: helpdesk@link.springer.de

2. Search Options

To search the LB data we recommend to use the LB search. The search engine has been tailored to suit your needs and offers the following search options:

- Search within the Tables of Contents, which also include the volume and subvolume titles **as well as the editor`s and authors names**
- Search within the full text of PDF documents
- Search within document titles only
- Search within **author names only**

For a refined search users may limit their search to a particular LB group.

If you wish to make a combined search of both the LB data collection as well as LINK then please use the LINK search.

No matter which search option you choose, you can limit the search to one or more groups. To reduce the number of results, a search refinement is possible.

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webmaster@springer.de

LB - Millennium Campaign

The LB Milllennium Campaign was the launch of a pre-release of LB online contents with

- full text PDFs available online
- excellent readability of table of contents
- clear and fast navigation in subvolumes with framestructure and java-script

Today more than 290 subvolumes of the unique, top-quality chemistry, physics and technology data collection are online available in LINK.

More than 10.000 users worldwide registered for the LB Millennium Campaign and took advantage of this first access point to electronic contents of LB.

Due to the overwhelming success, we decided to continue the Millennium Campaign until the end of 2001. This pre-release offers free trial access to the full text PDFs for selected parts of the LB online version. These contents are especially marked with FREE online in the different LB groups.

Access to the tables of contents and abstracts is free to everybody interested.

Placing the entire Landolt-Börnstein data collection online is a result of a readership survey where 83 % of LB readers and users said that they prefer the online version.

For further information on LB online licencing and registration terms please contact the LINK Helpdesk staff

North and South America, Canada: link@springer-ny.com
All other countries: helpdesk@link.springer.de

Landolt-Börnstein brings you the work of a thousand experts - right to your screen!

LB Catalog 2001

Contents

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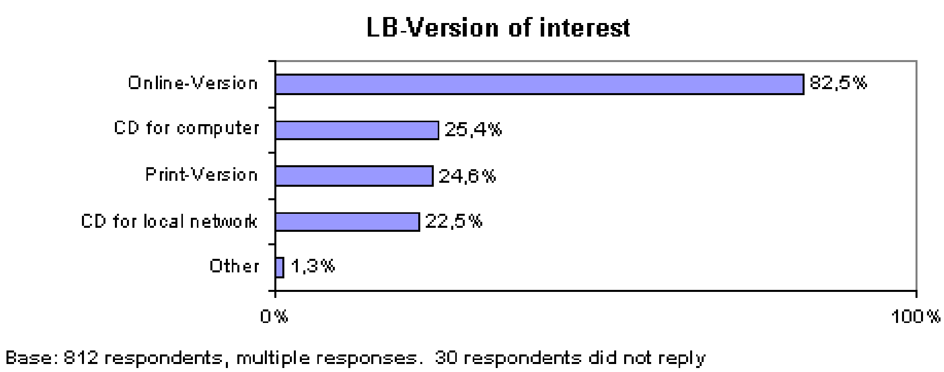
Readership Survey

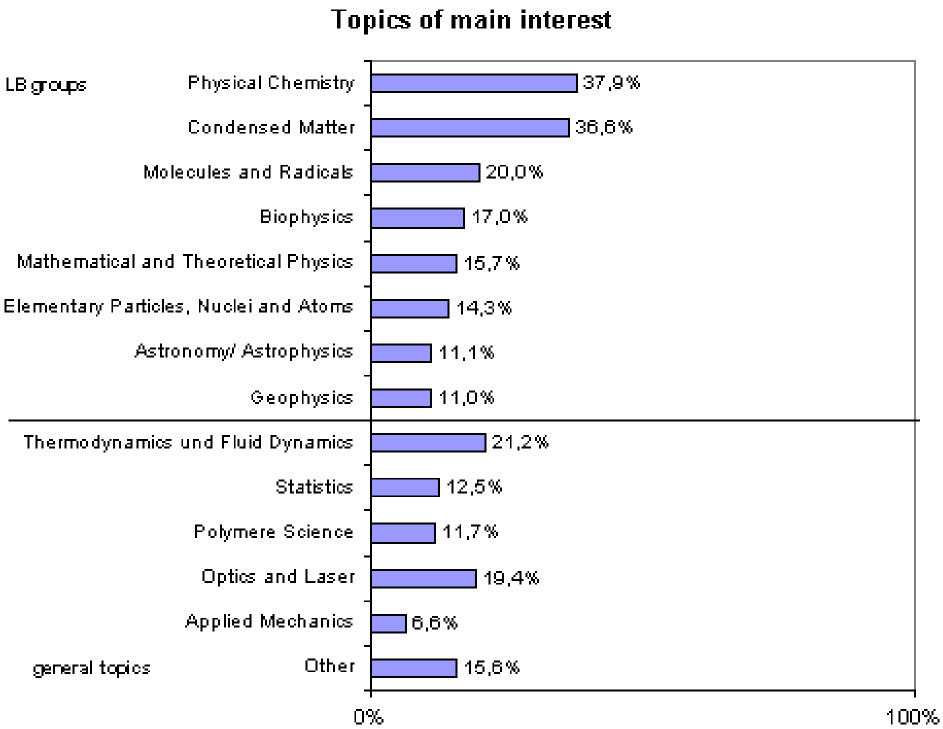
In January 2000 the Landolt-Börnstein Millennium Campaign was launched as an online pre-release. It provided free electronic access to a selected number of subvolumes. Within only 10 months 10.000 readers made use of this offer. This was a good reason for us to carry out a readership survey. The following graphics show the results of this survey:

Results of readership survey:

Q: **If you could choose, which version of the Landolt-Börnstein would you prefer?**
A: An overwhelming 83% said they would prefer using an online version.

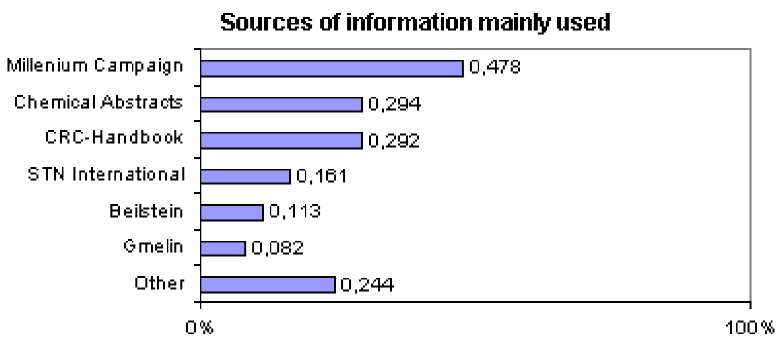


Q: **Which topics are of main interest to you?**
A: See graph below for results



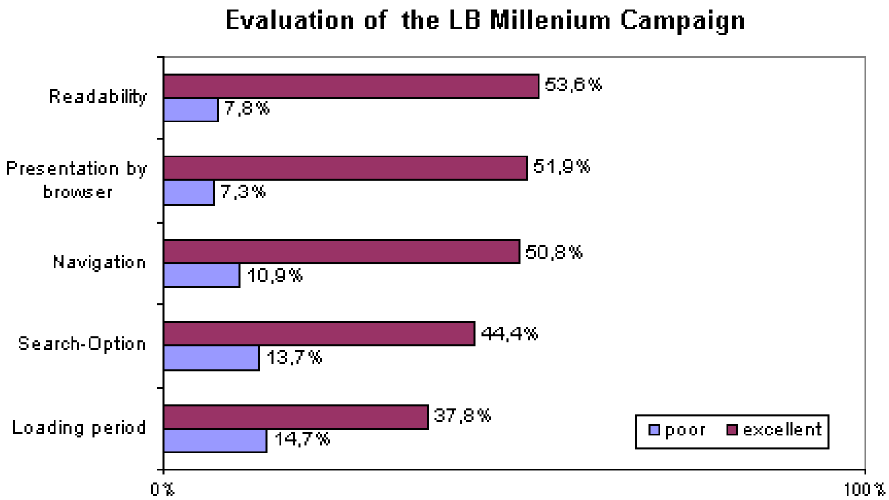
Base: 812 respondents, multiple responses. 28 respondents did not reply

Q: **Which databases do you mainly use for retrieving the information you are looking for?**
A: 47,8 % regarded Landolt-Börnstein as the most efficient information source.



Base: 812 respondents, multiple responses. 52 respondents did not reply

Q: **How did readers evaluate the readability, navigation, presentation, and search & loading time of Landolt-Börnstein's online version?**
A: They were mainly satisfied.



Base: 812 respondents, 135-109 (different for each criteria) respondents did not reply

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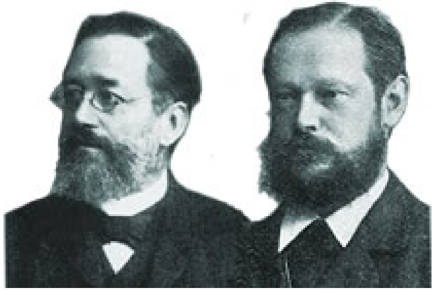
History of Landolt-Börnstein

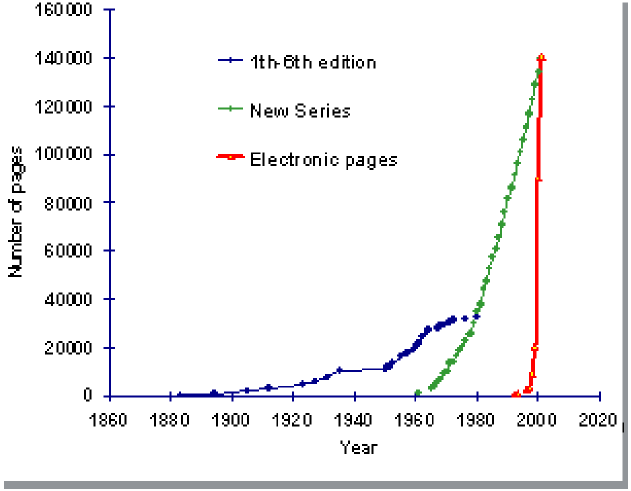


Hans Landolt 1831–1910 (Left)
Richard Börnstein 1852–1913 (Right)

H. Landolt, R. Börnstein and Julius Springer founded the Landolt- Börnstein data collection nearly 120 years ago in 1883. They recognized the need for selected and easily retrievable data at the scientist 's desk. Landolt's and Börnstein's idea now appears even more important than ever for 2 important reasons:

- due to the immense production rate of literature and data

Landolt-Börnstein, 1883-2001



- due to the steadily growing interdependence between increasingly differentiated research fields.

Today more than 1000 wellknown experts, working permanently as editors and authors for Landolt-Börnstein, supply the user with reliable data which otherwise could only be found with a great deal of effort, i.e. extensive individual full text literature research.

- regular supplementation on data fields of general importance

- adoption of new fields according to the needs of the user
- development of new electronic tool and complete electronic version to make Landolt Börnstein more real at the desk of the user and to improve the retrieval and document delivery procedures
- a Helpdesk on Internet is accessible

LANDOLT-BÖRNSTEIN

Numerical Data and Functional Relationships in Science and Technology

- All about Landolt-Börnstein
- Service and Orders

Landolt-Börnstein online on LINK:

- Landolt-Börnstein Contents
- Landolt-Börnstein Search

Springer

News

Landolt-Börnstein online with new release!

August 2002. We've just made LB Online even better! You'll be pleased to know that the latest version of LB Online now features a whole host of improvements. Much of the content has been revised. The navigation bar has been improved and now features hierarchically structured bookmarks for fast and easy orientation. And document, data files as well as the table of contents, substance and property files are now presented in PDF format. The powerful LB Search remains the best way to explore the collection's wealth of

Landolt-Börnstein: General Scientific Information and Tools

helpdesk@link.springer.de

Group IV

Physical Chemistry

Mechanical Properties

Electrical Properties

Thermodynamic Properties

LINK Helpdesk

Volumes of Group IV: Physical Chemistry

IV/8

Thermodynamic Properties of Organic Compounds and Their Mixtures

This volume provides temperatures and enthalpies of solid-solid and solid-liquid phase transitions, densities and vapor pressures of liquid organic compounds and their mixtures. All the values were critically evaluated. In each subvolume a Chemical Name Index and a Chemical Abstracts Service Registry Number (CASRN) Index for all compounds is also provided.

Subvolume A: Enthalpies of Fusion and Transition of Organic Compounds

1995. X, 588 pages. ISBN 3-540-58854-X

Editor: K.N. Marsh

Authors: Z.-Y. Zhang, M. Frenkel, K.N. Marsh, R.C. Wilhoit

Table of Contents including links to the full texts (PDF format)

Subvolume B: Densities of Aliphatic Hydrocarbon: Alkanes

1996. 119 figs., X, 410 pages. ISBN 3-540-61029-4

Editor: K.N. Marsh

Authors: R.C. Wilhoit, K.N. Marsh, X. Hong, N. Gadalla, M. Frenkel

Table of Contents including links to the full texts (PDF format)

Subvolume C: Densities of Aliphatic Hydrocarbon: Alkenes, Alkadienes, Alkynes, and Miscellaneous Compounds

1996. 78 figs., X, 381 pages. ISBN 3-540-61554-7

Editor: K.N. Marsh

Authors: R.C. Wilhoit, K.N. Marsh, X. Hong, N. Gadalla, M. Frenkel

Table of Contents including links to the full texts (PDF format)

Subvolume D: Densities of Monocyclic Hydrocarbons

1997. 117 figs., XIII, 466 pages, with CD-ROM. ISBN 3-540-62509-7

Editors: K.R. Hall, K.N. Marsh

Authors: R.C. Wilhoit, X. Hong, M. Frenkel, K.R. Hall

Table of Contents including links to the full texts (PDF format)

Subvolume E: Densities of Aromatic Hydrocarbons

1998. 79 figs., X, 373 pages, with CD-ROM. ISBN 3-540-62510-0

Editors: K.R. Hall, K.N. Marsh

Authors: R.C. Wilhoit, X. Hong, M. Frenkel, K.R. Hall

Table of Contents including links to the full texts (PDF format)

Subvolume F: Densities of Polycyclic Hydrocarbons

1999. 84 figs., XI, 538 pages, with CD-ROM. ISBN 3-540-65162-4

Editors: K.R. Hall, K.N. Marsh

Authors: R.C. Wilhoit, X. Hong, M. Frenkel, K.R. Hall

Table of Contents including links to the full texts (PDF format)

Subvolume G: Densities of Alcohols

2000. 110 figs., XI, 413 pages, with CD-ROM. ISBN 3-540-66233-2

Editors: K.R. Hall, K.N. Marsh

Authors: M. Frenkel, X. Hong, R.C. Wilhoit, K.R. Hall

Table of Contents including links to the full texts (PDF format)

Subvolume H: Densities of Esters and Ethers

2001. 105 figs., XI, 484 pages, with CD-ROM. ISBN 3-540-41035-X

Editors: K.R. Hall, K.N. Marsh

Authors: M. Frenkel, X. Hong, R.C. Wilhoit, K.R. Hall

Table of Contents including links to the full texts (PDF format)

Subvolume I: Densities of Phenols, Aldehydes, Ketones, Carboxylic Acids, Amines, Nitriles, and Nitrohydrocarbons

2002. 121 figs., X, 470 pages, with CD-ROM. ISBN 3-540-42883-6

Editors: M. Frenkel, K.N. Marsh

Authors: M. Frenkel, X. Hong, Q. Dong, X. Yan, R.D. Chirico

Table of Contents including links to the full texts (PDF format)

LINK Helpdesk

Contents

Phases		T/K	$\Delta_{trs}H$ /(kJ·mol^{-1})	Sample Description and Purity as %	Method	Reference
Bromotrichloromethane			**[75-62-7]**	**$CBrCl_3$**		MW = 198.27
cr	l	267.500 ± 0.02	2.531 ± 0.025	99.94m%		55-dre
Tetrabromomethane			**[558-13-4]**	**CBr_4**		MW = 331.63
cr,II	cr,I	320.05 ± 0.3	5.94 ± 0.1	cm;cs	drop	39-fre/hil
cr,II	cr,I	320.00 ± 0.2	6.669 ± 0.05	cm		56-mar/sta
cr,II	cr,I	320.15 ± 0.5	8.88 ± 0.17	ns	isoperibol	67-tse/god
cr,II	cr,I	320.0 ± 1.0	6.58 ± 0.08	cm;sb	DSC	70-sil/rud
cr,I	l	363.25 ± 0.3	3.95 ± 0.15	cm;cs	drop	39-fre/hil
cr,I	l	367.6 ± 1.0	3.56 ± 0.08	cm;sb	DSC	70-sil/rud
cr,I	l	364.05 ± 0.4		cm;cs	cryoscopic	48-van/dav
cr,I	l	365.15 ± 0.5				62-sha/wal
cr,II	cr,I	320.0 ± 1.0	6.62 ± 0.05			Selected
cr,I	l	365.4 ± 2.2	3.76 ± 0.19			Selected
Phosgene			**[75-44-5]**	**CCl_2O**		MW = 98.92
crm,II	l	139.19 ± 0.2	4.732 ± 0.06	sx; 99.963m%,hc	isoperibol	60-gia/ott
crm,I	l	142.09 ± 0.05	5.586 ± 0.04	sx; 99.963m%,hc	isoperibol	60-gia/ott
cr,I	l	145.370 ± 0.02	5.736 ± 0.010	cm;fd; 99.993m%,hc	isoperibol	48-gia/jon
Trichlorofluoromethane			**[75-69-4]**	**CCl_3F**		MW = 137.37
cr	l	162.68 ± 0.07	6.894 ± 0.017	cm;fd,dc,av; 99.95m%,hc		41-osb/gar
cr	l	162.670 ± 0.05		cm;fd; 99.95m%,ta	cryoscopic	64-ott/goa
cr	l	165.40 ± 0.2	7.90 ± 0.16		DSC	82-mar
cr	l	162.720 ± 0.010		cm;fd; 99.89m%,ta		87-ott/woo
cr	l	162.704 ± 0.010		ns;99.99%		91-bla/wei
cr	l	162.195 ± 0.05		cm;ns; 99.85w%,glc		92-men/cha
cr	l	162.69 ± 0.06		cm;ns; 99.85w%,glc		92-men/cha
cr	l	162.68 ± 0.06		cm;ns; 99.85w%,glc		92-men/cha
cr	l	162.688 ± 0.03		cm;ns; 99.85w%,glc		92-men/cha
cr	l	162.659 ± 0.02		cm;ns; 99.85w%,glc		92-men/cha

Trichlorofluoromethane *(cont.)*

Phases		T/K	$\Delta_{trs}H$ /(kJ·mol^{-1})	Sample Description and Purity as %	Method	Reference
cr	l	162.695 ± 0.03		cm;ns; 99.85w%,glc		92-men/cha
cr	l	162.71 ± 0.02	6.894 ± 0.017			Selected
Trichloronitromethane			**[76-06-2]**	**CCl_3NO_2**		MW = 164.37
cr	l	203.660 ± 0.02	11.54 ± 0.12	99.65m%		55-dre
Tetrachloromethane			**[56-23-5]**	**CCl_4**		MW = 153.82
cr,II	cr,I	224.60 ± 0.2	4.600 ± 0.05			22-lat
cr,II	cr,I	225.489 ± 0.05	4.522 ± 0.021			34-joh/lon
cr,II	cr,I	225.63 ± 0.2	4.60 ± 0.21			37-stu
cr,II	cr,I	225.350 ± 0.05	4.581 ± 0.033			44-hic/hoo
cr,II	cr,I	225.350 ± 0.05	2.515 ± 0.05	xx	isoperibol	44-hic/hoo
cr,II	cr,I	225.75 ± 0.10	4.59 ± 0.21	ns	adiabatic	49-sta/gup
cr,II	cr,I	225.10 ± 0.5	4.47 ± 0.17	ns		67-gra-1
cr,II	cr,I	226.6 ± 1.0	4.46 ± 0.33	cm;fd; >99.95%	DSC	70-sil/rud
cr,II	cr,I	225.32 ± 0.10	4.745 ± 0.042			71-bag/man
cr,II	cr,I	225.7 ± 0.2	4.631 ± 0.010	cm; 99.993m%,hc	adiabatic	76-mor/ric
cr,I	crm	234.30 ± 0.5	0.68 ± 0.08	ns		67-gra-1
crm	l	245.4 ± 1.0	1.76 ± 0.08	ns		67-gra-1
crm	l	245.0 ± 1.0	1.72 ± 0.13	cm;fd; >99.95%	DSC	70-sil/rud
crm	l	245.700 ± 0.02	1.848 ± 0.006	cm;fc; 99.97m%,ta	adiabatic	72-are/mil
crm	l	246.000 ± 0.02	1.830 ± 0.010	cm; 99.993m%,hc	adiabatic	76-mor/ric
cr,I	l	248.45 ± 0.20	2.648 ± 0.10			10-bec/wae
cr,I	l	249.0 ± 1.0	2.694 ± 0.05			22-lat
cr,I	l	250.280 ± 0.05	2.415 ± 0.021			34-joh/lon
cr,I	l	250.37 ± 0.2	2.43 ± 0.08			37-stu
cr,I	l	250.30 ± 0.15	2.515 ± 0.025			44-hic/hoo
cr,I	l	250.0 ± 1.5	2.552 ± 0.034			39-van
cr,I	l		4.581 ± 0.05	xx	isoperibol	44-hic/hoo
cr,I	l	250.20 ± 0.2	2.52 ± 0.13	ns	adiabatic	49-stag/up
cr,I	l	250.30 ± 0.5	2.51 ± 0.08	ns		67-gra-1
cr,I	l	247.8 ± 1.0	2.49 ± 0.13	cm;fd; >99.95%	DSC	70-sil/rud
cr,I	l	250.280 ± 0.02	2.558 ± 0.010	cm;fc; 99.97m%,ta	adiabatic	72-are/mil
cr,I	l	250.530 ± 0.02	2.562 ± 0.010	cm; 99.993m%,hc	adiabatic	76-mor/ric

Tetrachloromethane *(cont.)*

Methane **[74-82-8]** **CH_4** **MW = 16.0428** **1**

T_c = 190.56 K [95-amb/tso]
ρ_c = 162.70 kg·m^{-3} [95-amb/tso]

Table 1. Coefficients for the polynomial expansion equations. Standard deviations (see introduction): $\sigma_\ell = 1.2258 \cdot 10^{-1}$ (low temperature range), $\sigma_{c,w} = 1.8083 \cdot 10^{-1}$ (combined temperature ranges, weighted), $\sigma_{c,uw} = 2.8956 \cdot 10^{-2}$ (combined temperature ranges, unweighted).

Coefficient	T = 90.69 to 158.00 K $\rho = A + BT + CT^2 + DT^3 + \ldots$	T = 158.00 to 190.56 K $\rho = [1 + 1.75(1 - T/T_c)^{1/3} + 0.75(1 - T/T_c)]$ $[\rho_c + A(T_c - T) + B(T_c - T)^2 + C(T_c - T)^3$ $+ D(T_c - T)^4]$
A	$5.31752 \cdot 10^{2}$	$-4.25250 \cdot 10^{-1}$
B	$-2.19382 \cdot 10^{-4}$	$4.30138 \cdot 10^{-2}$
C	$-1.76410 \cdot 10^{-2}$	$-1.43130 \cdot 10^{-3}$
D	$1.18522 \cdot 10^{-4}$	$1.55893 \cdot 10^{-5}$
E	$-3.49068 \cdot 10^{-7}$	

Table 2. Experimental values with uncertainties and deviation from calculated values.

$\frac{T}{K}$	$\frac{\rho_{exp} \pm 2\sigma_{est}}{kg \cdot m^{-3}}$	$\frac{\rho_{exp} - \rho_{calc}}{kg \cdot m^{-3}}$	Ref. (Symbol in Fig. 1)	$\frac{T}{K}$	$\frac{\rho_{exp} \pm 2\sigma_{est}}{kg \cdot m^{-3}}$	$\frac{\rho_{exp} - \rho_{calc}}{kg \cdot m^{-3}}$	Ref. (Symbol in Fig. 1)
	crystal II			77.40	494.2 ± 0.8		64-man/tol[1)]
20.06	524.8 ± 1.4		30-heu[1)]	85.40	489.2 ± 0.8		64-man/tol[1)]
20.13	524.8 ± 1.0		30-heu[1)]	20.40	522.5 ± 0.8		66-tol/man[1)]
20.20	524.6 ± 1.0		30-heu[1)]	90.67	517.0 ± 10.0		67-gue/ric[1)]
20.27	523.8 ± 1.0		30-heu[1)]		*liquid*		
20.30	524.4 ± 1.0		30-heu[1)]	183.15	264.30 ± 0.25	2.52	62-shi/koh[1)]
20.35	523.9 ± 1.0		30-heu[1)]	138.96	379.01 ± 0.30	0.06	65-ven[1)]
20.37	523.5 ± 1.0		30-heu[1)]	149.77	360.01 ± 0.30	1.45	65-ven[1)]
20.42	523.6 ± 1.0		30-heu[1)]	158.82	340.67 ± 0.30	1.21	65-ven(✕)
20.45	523.4 ± 1.0		30-heu[1)]	166.75	320.98 ± 0.30	0.78	65-ven(✕)
20.48	523.4 ± 1.0		30-heu[1)]	174.75	296.81 ± 0.30	0.98	65-ven(✕)
20.52	523.5 ± 1.0		30-heu[1)]	178.70	281.86 ± 0.30	0.58	65-ven[1)]
20.56	523.4 ± 1.0		30-heu[1)]	182.58	265.15 ± 0.40	0.61	65-ven[1)]
20.63	523.5 ± 1.0		30-heu[1)]	186.74	240.25 ± 0.00	-0.67	65-ven[1)]
20.73	523.9 ± 1.0		30-heu[1)]	188.82	220.67 ± 0.00	-1.85	65-ven[1)]
	crystal I			189.85	206.44 ± 0.00	-0.58	65-ven[1)]
20.11	524.2 ± 1.0		30-heu[1)]	93.51	447.75 ± 0.06	0.05	72-goo/pry(○)
20.17	524.2 ± 1.0		30-heu[1)]	97.17	442.86 ± 0.06	0.07	72-goo/pry(○)
20.23	778.9 ± 2.0		30-heu[1)]	101.43	437.05 ± 0.06	0.08	72-goo/pry(○)
20.34	523.9 ± 1.0		30-heu[1)]	105.17	431.81 ± 0.06	0.04	72-goo/pry(○)
20.43	523.6 ± 1.0		30-heu[1)]	109.61	425.57 ± 0.06	0.09	72-goo/pry(○)
20.50	523.5 ± 1.0		30-heu[1)]	113.77	419.45 ± 0.05	0.01	72-goo/pry(○)
20.66	523.5 ± 1.0		30-heu[1)]	117.75	413.61 ± 0.05	0.08	72-goo/pry(○)
20.80	523.5 ± 1.0		30-heu[1)]	121.89	407.29 ± 0.05	0.07	72-goo/pry(○)
20.86	523.4 ± 1.0		30-heu[1)]	125.82	401.05 ± 0.05	-0.00	72-goo/pry(○)
90.67	518.5 ± 6.7		40-clu/wei[1)]	129.66	394.83 ± 0.05	-0.02	72-goo/pry(○)
77.00	507.0 ± 5.0		58-lar[1)]	133.77	388.01 ± 0.05	0.03	72-goo/pry(○)

[1)] Not included in Fig. 1.

cont.

Methane (cont.)

Table 2. (cont.)

$\frac{T}{K}$	$\frac{\rho_{exp} \pm 2\sigma_{est}}{kg \cdot m^{-3}}$	$\frac{\rho_{exp} - \rho_{calc}}{kg \cdot m^{-3}}$	Ref. (Symbol in Fig. 1)	$\frac{T}{K}$	$\frac{\rho_{exp} \pm 2\sigma_{est}}{kg \cdot m^{-3}}$	$\frac{\rho_{exp} - \rho_{calc}}{kg \cdot m^{-3}}$	Ref. (Symbol in Fig. 1)
133.88	387.85 ± 0.05	0.05	72-goo/pry(○)	123.15	405.27 ± 0.10	0.01	76-mcc[1)]
139.35	378.26 ± 0.05	0.01	72-goo/pry(○)	105.00	432.29 ± 0.07	0.28	77-hay/hiz(□)
145.45	367.06 ± 0.05	0.07	72-goo/pry(○)	110.00	425.11 ± 0.07	0.19	77-hay/hiz(□)
151.55	355.03 ± 0.06	0.07	72-goo/pry(○)	115.00	417.82 ± 0.07	0.19	77-hay/hiz(□)
157.20	342.98 ± 0.07	-0.05	72-goo/pry(○)	120.00	410.25 ± 0.05	0.13	77-hay/hiz(□)
163.70	327.72 ± 0.08	-0.34	72-goo/pry(○)	125.00	402.42 ± 0.05	0.07	77-hay/hiz(□)
169.33	312.71 ± 0.10	-0.27	72-goo/pry(○)	130.00	394.29 ± 0.05	0.00	77-hay/hiz(□)
175.05	295.03 ± 0.13	0.24	72-goo/pry(○)	135.00	385.89 ± 0.05	0.01	77-hay/hiz(□)
95.00	445.81 ± 0.10	0.10	75-ols[1)]	140.00	377.11 ± 0.05	0.02	77-hay/hiz(□)
100.00	439.19 ± 0.10	0.25	75-ols[1)]	145.00	367.88 ± 0.06	0.04	77-hay/hiz(□)
105.00	432.10 ± 0.10	0.09	75-ols[1)]	150.00	358.10 ± 0.06	0.00	77-hay/hiz(□)
110.00	424.99 ± 0.10	0.07	75-ols[1)]	160.00	336.70 ± 0.06	-0.11	77-hay/hiz(□)
115.00	417.67 ± 0.10	0.04	75-ols[1)]	91.00	451.03 ± 0.06	0.01	86-kle/wag(◆)
120.00	409.99 ± 0.10	-0.13	75-ols[1)]	91.00	451.05 ± 0.06	0.03	86-kle/wag(◆)
125.00	402.37 ± 0.10	0.02	75-ols[1)]	95.00	445.69 ± 0.06	-0.02	86-kle/wag(◆)
130.00	394.30 ± 0.10	0.01	75-ols[1)]	100.00	438.89 ± 0.06	-0.05	86-kle/wag(◆)
135.00	385.91 ± 0.10	0.03	75-ols[1)]	103.00	434.73 ± 0.06	-0.07	86-kle/wag(◆)
140.00	377.13 ± 0.10	0.04	75-ols[1)]	105.00	431.92 ± 0.06	-0.09	86-kle/wag(◆)
145.00	367.91 ± 0.10	0.07	75-ols[1)]	110.00	424.77 ± 0.06	-0.15	86-kle/wag(◆)
150.00	358.15 ± 0.10	0.05	75-ols(✕)	111.63	422.40 ± 0.07	-0.17	86-kle/wag(◆)
155.00	347.77 ± 0.10	-0.00	75-ols(✕)	111.63	422.38 ± 0.07	-0.19	86-kle/wag(◆)
160.00	336.58 ± 0.12	-0.23	75-ols(✕)	115.00	417.43 ± 0.07	-0.20	86-kle/wag(◆)
165.00	324.37 ± 0.15	-0.42	75-ols(✕)	116.00	415.95 ± 0.07	-0.20	86-kle/wag(◆)
170.00	310.76 ± 0.18	-0.25	75-ols(✕)	120.00	409.89 ± 0.08	-0.23	86-kle/wag[1)]
175.00	295.20 ± 0.19	0.24	75-ols(✕)	120.00	409.88 ± 0.08	-0.24	86-kle/wag[1)]
178.00	284.45 ± 0.19	0.44	75-ols(✕)	125.00	402.08 ± 0.08	-0.27	86-kle/wag[1)]
180.00	284.45 ± 0.19	8.45	75-ols[1)]	130.00	394.01 ± 0.07	-0.28	86-kle/wag(◆)
181.00	272.12 ± 0.19	0.38	75-ols(✕)	135.00	385.01 ± 0.07	-0.87	86-kle/wag[1)]
182.00	267.51 ± 0.21	0.25	75-ols(✕)	140.00	376.84 ± 0.10	-0.25	86-kle/wag[1)]
183.00	262.59 ± 0.21	0.08	75-ols(✕)	140.00	376.83 ± 0.07	-0.26	86-kle/wag(◆)
184.00	257.26 ± 0.22	-0.19	75-ols(✕)	145.00	367.62 ± 0.10	-0.22	86-kle/wag[1)]
185.00	251.44 ± 0.24	-0.52	75-ols(✕)	150.00	357.87 ± 0.13	-0.23	86-kle/wag[1)]
186.00	244.96 ± 0.24	-0.95	75-ols(✕)	155.00	347.49 ± 0.16	-0.28	86-kle/wag[1)]
187.00	237.56 ± 0.00	-1.47	75-ols[1)]	160.00	336.28 ± 0.20	-0.53	86-kle/wag(◆)
188.00	228.77 ± 0.00	-2.11	75-ols[1)]	160.00	336.29 ± 0.20	-0.52	86-kle/wag(◆)
189.00	217.56 ± 0.00	-2.81	75-ols[1)]	160.00	336.30 ± 0.20	-0.51	86-kle/wag(◆)
189.40	211.78 ± 0.00	-3.13	75-ols[1)]	165.00	324.07 ± 0.30	-0.72	86-kle/wag(◆)
93.13	448.39 ± 0.10	0.19	76-mcc(∇)	170.00	310.46 ± 0.30	-0.55	86-kle/wag(◆)
98.15	441.61 ± 0.10	0.15	76-mcc[1)]	175.00	294.89 ± 0.20	-0.07	86-kle/wag(◆)
103.15	434.73 ± 0.10	0.14	76-mcc[1)]	180.00	276.18 ± 0.20	0.18	86-kle/wag(◆)
108.15	427.58 ± 0.10	0.02	76-mcc[1)]	180.00	276.19 ± 0.20	0.19	86-kle/wag(◆)
113.15	420.29 ± 0.10	-0.06	76-mcc[1)]	180.00	276.18 ± 0.20	0.18	86-kle/wag(◆)
118.15	412.85 ± 0.10	-0.08	76-mcc[1)]	182.00	267.28 ± 0.20	0.02	86-kle/wag(◆)

[1)] Not included in Fig. 1.

cont.

Methane (cont.)

Table 2. (cont.)

$\frac{T}{K}$	$\frac{\rho_{exp} \pm 2\sigma_{est}}{kg \cdot m^{-3}}$	$\frac{\rho_{exp} - \rho_{calc}}{kg \cdot m^{-3}}$	Ref. (Symbol in Fig. 1)	$\frac{T}{K}$	$\frac{\rho_{exp} \pm 2\sigma_{est}}{kg \cdot m^{-3}}$	$\frac{\rho_{exp} - \rho_{calc}}{kg \cdot m^{-3}}$	Ref. (Symbol in Fig. 1)
184.00	257.07 ± 0.20	-0.38	86-kle/wag(◆)	190.00	200.47 ± 0.00	-3.19	86-kle/wag[1)]
186.00	244.83 ± 0.20	-1.08	86-kle/wag(◆)	190.10	197.85 ± 0.00	-3.22	86-kle/wag[1)]
186.00	244.84 ± 0.20	-1.07	86-kle/wag(◆)	190.20	194.82 ± 0.00	-3.26	86-kle/wag[1)]
187.00	237.49 ± 0.00	-1.54	86-kle/wag[1)]	190.30	191.20 ± 0.00	-3.28	86-kle/wag[1)]
187.00	237.50 ± 0.00	-1.53	86-kle/wag[1)]	190.40	186.46 ± 0.00	-3.35	86-kle/wag[1)]
188.00	228.80 ± 0.00	-2.08	86-kle/wag[1)]	190.45	183.28 ± 0.00	-3.43	86-kle/wag[1)]
188.00	228.81 ± 0.00	-2.07	86-kle/wag[1)]	190.50	178.87 ± 0.00	-3.63	86-kle/wag[1)]
189.00	217.71 ± 0.00	-2.66	86-kle/wag[1)]	190.53	174.68 ± 0.00	-4.05	86-kle/wag[1)]
189.50	210.41 ± 0.00	-2.95	86-kle/wag[1)]	90.69	451.25 ± 0.08	-0.18	89-fri/ely(Δ)
189.80	204.94 ± 0.00	-3.10	86-kle/wag[1)]				

[1)] Not included in Fig. 1.

Further references: [15-car-2, 22-key/tay, 40-clu/wei, 45-cor/bow, 53-blo/par, 56-mat/sta, 58-cro/sco, 62-mor, 64-cro/sco, 64-kno/abb, 65-fuk/leg, 66-dav/row, 67-gil/zwi, 67-gue/ric, 68-sha/can, 69-jen/kur, 69-ric/sca, 69-ter/lyn, 70-jan/gie, 71-cal/sta, 71-str, 72-liu/mil, 73-rod/mil, 74-goo, 76-hay/hiz-1, 76-nun/sta, 77-orr/lau, 78-ang/arm, 87-you/ely, 96-wag/der].

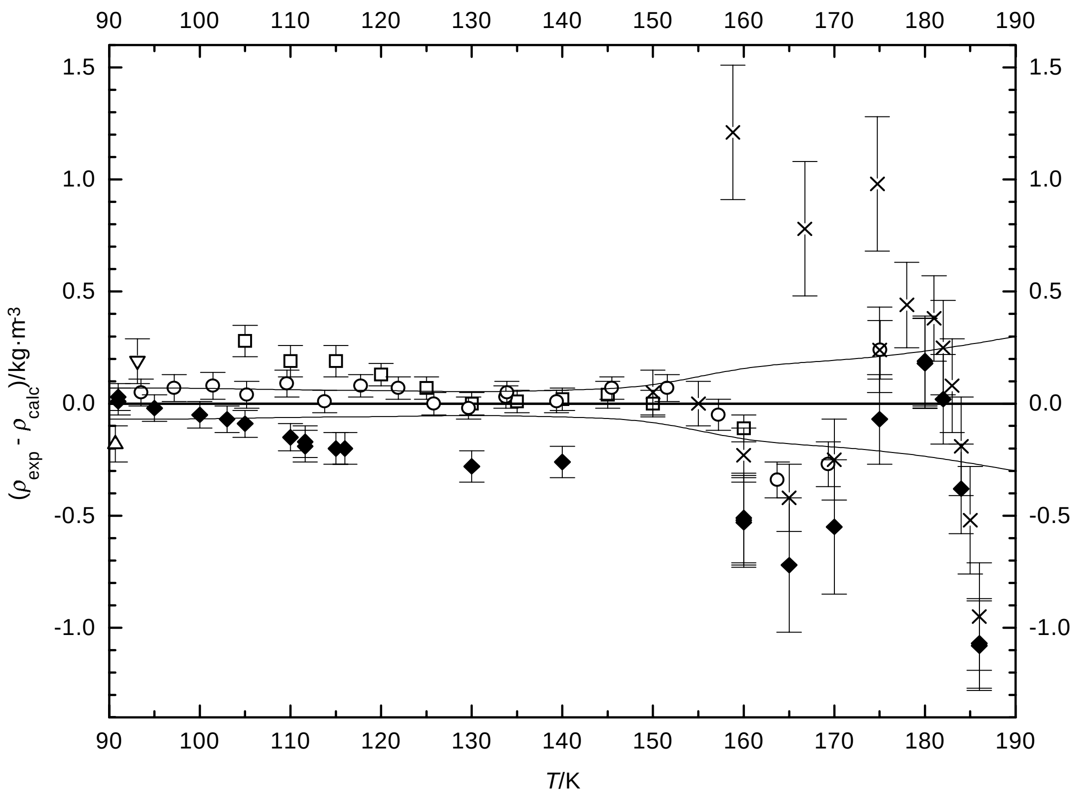


Fig. 1. The symbols show the deviation of the calculated from the experimental values from Table 2. The curves above and below the zero line indicate the calculated error region of the recommended values given in Table 3. The error bars are the experimental uncertainties. (Error bars smaller than the symbols are omitted to clarify the figure.)

cont.

Methane (cont.)

Table 3. Recommended values (fit to the reliable experimental values according to the equations
$\rho = A + BT + CT^2 + DT^3 + \ldots$ or $\rho = [1 + 1.75(1 - T/T_c)^{1/3} + 0.75(1 - T/T_c)][\rho_c + A(T_c - T) + B(T_c - T)^2 + C(T_c - T)^3 + D(T_c - T)^4]$).

$\frac{T}{K}$	$\frac{\rho \pm \sigma_{fit}}{kg \cdot m^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{fit}}{kg \cdot m^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{fit}}{kg \cdot m^{-3}}$
	crystal II		*liquid*	140.00	377.09 ± 0.06
20.52	523.5	90.00	452.34 ± 0.07	150.00	358.10 ± 0.07
	crystal I	100.00	438.94 ± 0.07	160.00	336.81 ± 0.17
20.52	523.5	110.00	424.92 ± 0.06	170.00	311.01 ± 0.19
80.00	492.6	120.00	410.12 ± 0.06	180.00	276.00 ± 0.23
		130.00	394.29 ± 0.05	190.00	203.66 ± 0.30

Ethane **[74-84-0]** **C_2H_6** **MW = 30.0696** **2**

T_c = 305.32 K [95-amb/tso]
ρ_c = 206.60 kg·m^{-3} [95-amb/tso]

Table 1. Coefficients for the polynomial expansion equations. Standard deviations (see introduction): $\sigma_\ell = 6.6316 \cdot 10^{-1}$ (low temperature range), $\sigma_{c,w} = 5.5091 \cdot 10^{-1}$ (combined temperature ranges, weighted), $\sigma_{c,uw} = 3.7510 \cdot 10^{-2}$ (combined temperature ranges, unweighted).

Coefficient	T = 90.35 to 250.00 K $\rho = A + BT + CT^2 + DT^3 + \ldots$	T = 250.00 to 305.32 K $\rho = [1 + 1.75(1 - T/T_c)^{1/3} + 0.75(1 - T/T_c)]$ $[\rho_c + A(T_c - T) + B(T_c - T)^2 + C(T_c - T)^3 + D(T_c - T)^4]$
A	$7.25893 \cdot 10^{2}$	$1.73573 \cdot 10^{-1}$
B	$-4.21275 \cdot 10^{-1}$	$-1.97578 \cdot 10^{-3}$
C	$-6.84937 \cdot 10^{-3}$	$2.60345 \cdot 10^{-6}$
D	$3.22751 \cdot 10^{-5}$	$2.71285 \cdot 10^{-8}$
E	$-6.36130 \cdot 10^{-8}$	

Table 2. Experimental values with uncertainties and deviation from calculated values.

$\frac{T}{K}$	$\frac{\rho_{exp} \pm 2\sigma_{est}}{kg \cdot m^{-3}}$	$\frac{\rho_{exp} - \rho_{calc}}{kg \cdot m^{-3}}$	Ref. (Symbol in Fig. 1)	$\frac{T}{K}$	$\frac{\rho_{exp} \pm 2\sigma_{est}}{kg \cdot m^{-3}}$	$\frac{\rho_{exp} - \rho_{calc}}{kg \cdot m^{-3}}$	Ref. (Symbol in Fig. 1)
	crystal III			295.67	327.73 ± 0.16	-0.43	69-sli(○)
20.00	759.3 ± 9.6		30-heu[1)]	298.17	314.89 ± 0.20	-0.51	69-sli(○)
20.00	751.7 ± 9.4		30-heu[1)]	300.66	298.80 ± 0.30	-0.96	69-sli(○)
20.00	749.9 ± 9.3		30-heu[1)]	302.16	286.68 ± 0.35	-1.05	69-sli(○)
77.00	713.0 ± 1.0		58-ste/lar[1)]	303.16	276.34 ± 0.40	-1.25	69-sli(○)
	liquid			304.15	262.56 ± 0.45	-1.47	69-sli(○)
108.15	632.27 ± 0.30	-0.07	68-sha/can(∇)	304.65	252.50 ± 0.50	-1.56	69-sli[1)]
283.20	373.55 ± 0.15	-0.18	69-sli(○)	305.15	235.37 ± 0.00	-1.09	69-sli[1)]
288.19	357.68 ± 0.15	-0.15	69-sli(○)	283.20	373.90 ± 0.12	0.17	71-tom(□)
293.18	338.90 ± 0.15	-0.23	69-sli(○)	288.19	358.10 ± 0.12	0.27	71-tom(□)

1) Not included in Fig. 1.

cont.

Ethane (cont.)

Table 2. (cont.)

$\frac{T}{K}$	$\frac{\rho_{exp} \pm 2\sigma_{est}}{kg \cdot m^{-3}}$	$\frac{\rho_{exp} - \rho_{calc}}{kg \cdot m^{-3}}$	Ref. (Symbol in Fig. 1)	$\frac{T}{K}$	$\frac{\rho_{exp} \pm 2\sigma_{est}}{kg \cdot m^{-3}}$	$\frac{\rho_{exp} - \rho_{calc}}{kg \cdot m^{-3}}$	Ref. (Symbol in Fig. 1)
299.85	306.60 ± 0.40	1.31	73-kah[1)]	158.15	576.09 ± 0.40	0.26	76-mcc(✕)
299.85	306.30 ± 0.40	1.01	73-kah[1)]	163.15	570.24 ± 0.40	0.30	76-mcc(✕)
91.01	650.69 ± 0.42	-0.10	73-rod/mil(✕)	168.15	564.26 ± 0.40	0.27	76-mcc(✕)
100.02	640.87 ± 0.41	-0.29	73-rod/mil(✕)	173.15	558.25 ± 0.40	0.28	76-mcc[1)]
108.11	632.21 ± 0.40	-0.18	73-rod/mil[1)]	215.77	503.75 ± 0.29	1.30	76-pal/pop(◆)
115.05	624.59 ± 0.39	-0.18	73-rod/mil(✕)	223.50	493.83 ± 0.29	2.63	76-pal/pop[1)]
93.15	648.54 ± 0.40	0.02	76-mcc(✕)	230.49	482.14 ± 0.29	1.55	76-pal/pop(◆)
98.15	643.14 ± 0.40	-0.04	76-mcc(✕)	241.20	464.69 ± 0.29	1.30	76-pal/pop(◆)
103.15	637.74 ± 0.40	-0.04	76-mcc(✕)	248.48	452.51 ± 0.29	1.54	76-pal/pop(◆)
108.15	632.30 ± 0.40	-0.04	76-mcc[1)]	256.49	437.63 ± 0.29	1.26	76-pal/pop(◆)
293.18	339.50 ± 0.20	0.37	71-tom(□)	268.41	412.41 ± 0.29	0.69	76-pal/pop(◆)
295.67	328.50 ± 0.25	0.34	71-tom(□)	277.86	390.56 ± 0.29	1.84	76-pal/pop(◆)
298.17	315.80 ± 0.30	0.40	71-tom(□)	292.74	342.08 ± 0.31	1.15	76-pal/pop(◆)
300.66	300.10 ± 0.40	0.34	71-tom[1)]	301.73	291.34 ± 0.39	-0.14	76-pal/pop(◆)
302.16	288.00 ± 0.50	0.27	71-tom[1)]	304.04	264.93 ± 0.46	-0.90	76-pal/pop[1)]
248.15	452.76 ± 0.30	1.21	73-dou/har(✕)	100.00	641.71 ± 0.39	0.52	77-hay/hiz(Δ)
253.15	443.62 ± 0.30	1.00	73-dou/har(✕)	105.00	636.23 ± 0.39	0.46	77-hay/hiz(Δ)
263.15	423.65 ± 0.30	0.55	73-dou/har(✕)	110.00	630.70 ± 0.39	0.38	77-hay/hiz[1)]
273.15	401.19 ± 0.30	0.53	73-dou/har(✕)	115.00	625.23 ± 0.39	0.41	77-hay/hiz(Δ)
283.15	374.61 ± 0.30	0.73	73-dou/har(✕)	120.00	619.50 ± 0.39	0.21	77-hay/hiz(Δ)
293.15	339.70 ± 0.30	0.45	73-dou/har(✕)	125.00	613.98 ± 0.38	0.26	77-hay/hiz(Δ)
298.15	315.70 ± 0.35	0.19	73-dou/har(✕)	130.00	608.36 ± 0.37	0.25	77-hay/hiz(Δ)
302.15	286.98 ± 0.40	-0.84	73-dou/har(✕)	135.00	602.78 ± 0.36	0.31	77-hay/hiz(Δ)
303.15	276.94 ± 0.45	-0.77	73-dou/har[1)]	140.00	597.08 ± 0.35	0.29	77-hay/hiz(Δ)
304.15	262.72 ± 0.56	-1.31	73-dou/har[1)]	150.00	585.61 ± 0.34	0.29	77-hay/hiz(Δ)
305.15	235.45 ± 0.00	-1.01	73-dou/har[1)]	160.00	573.90 ± 0.32	0.25	77-hay/hiz(Δ)
305.25	228.53 ± 0.00	-0.25	73-dou/har[1)]	170.00	561.90 ± 0.30	0.13	77-hay/hiz(Δ)
266.45	413.30 ± 0.40	-2.76	73-kah[1)]	180.00	549.65 ± 0.28	0.06	77-hay/hiz(Δ)
277.55	389.80 ± 0.40	0.26	73-kah(✕)	190.00	537.08 ± 0.26	0.02	77-hay/hiz(Δ)
288.75	356.40 ± 0.40	0.51	73-kah[1)]	200.00	524.08 ± 0.24	-0.00	77-hay/hiz(Δ)
288.75	356.20 ± 0.40	0.31	73-kah[1)]	210.00	510.32 ± 0.22	-0.23	77-hay/hiz(Δ)
294.25	335.90 ± 0.40	1.31	73-kah[1)]	220.00	496.11 ± 0.20	-0.24	77-hay/hiz(Δ)
294.25	335.40 ± 0.45	0.81	73-kah[1)]	230.00	481.03 ± 0.18	-0.31	77-hay/hiz(Δ)
113.15	626.84 ± 0.40	-0.02	76-mcc[1)]	240.00	465.00 ± 0.16	-0.38	77-hay/hiz(Δ)
118.15	621.29 ± 0.40	-0.05	76-mcc(✕)	250.00	447.73 ± 0.13	-0.57	77-hay/hiz(Δ)
123.15	615.72 ± 0.40	-0.06	76-mcc(✕)	260.00	428.82 ± 0.12	-0.70	77-hay/hiz(Δ)
128.15	610.14 ± 0.40	-0.05	76-mcc(✕)	270.00	407.42 ± 0.11	-0.69	77-hay/hiz(Δ)
133.15	604.56 ± 0.40	-0.00	76-mcc(✕)	102.58	638.40 ± 0.34	0.00	77-orr/lau(✕)
138.15	599.03 ± 0.40	0.13	76-mcc(✕)	103.71	637.06 ± 0.34	-0.12	77-orr/lau(✕)
143.15	593.52 ± 0.40	0.33	76-mcc(✕)	106.17	634.25 ± 0.35	-0.25	77-orr/lau(✕)
148.15	587.77 ± 0.40	0.32	76-mcc(✕)	108.93	631.22 ± 0.35	-0.27	77-orr/lau(✕)
153.15	581.97 ± 0.40	0.31	76-mcc(✕)	111.49	628.39 ± 0.35	-0.30	77-orr/lau(✕)

[1)] Not included in Fig. 1.

cont.

Ethane (cont.)

Table 2. (cont.)

$\frac{T}{K}$	$\frac{\rho_{exp} \pm 2\sigma_{est}}{kg \cdot m^{-3}}$	$\frac{\rho_{exp} - \rho_{calc}}{kg \cdot m^{-3}}$	Ref. (Symbol in Fig. 1)	$\frac{T}{K}$	$\frac{\rho_{exp} \pm 2\sigma_{est}}{kg \cdot m^{-3}}$	$\frac{\rho_{exp} - \rho_{calc}}{kg \cdot m^{-3}}$	Ref. (Symbol in Fig. 1)
114.22	625.32 ± 0.35	-0.36	77-orr/lau(✕)	171.34	559.92 ± 0.41	-0.23	77-orr/lau[1)]
117.00	622.48 ± 0.36	-0.13	77-orr/lau(✕)	174.11	556.58 ± 0.41	-0.22	77-orr/lau[1)]
119.62	619.43 ± 0.36	-0.28	77-orr/lau(✕)	176.87	553.24 ± 0.42	-0.20	77-orr/lau[1)]
122.30	616.38 ± 0.36	-0.35	77-orr/lau(✕)	179.60	549.78 ± 0.42	-0.31	77-orr/lau[1)]
125.00	613.44 ± 0.37	-0.28	77-orr/lau(✕)	182.42	546.22 ± 0.42	-0.38	77-orr/lau(✕)
127.68	610.51 ± 0.37	-0.21	77-orr/lau(✕)	185.16	543.05 ± 0.43	-0.13	77-orr/lau(✕)
130.32	607.59 ± 0.37	-0.16	77-orr/lau(✕)	187.95	539.35 ± 0.43	-0.31	77-orr/lau(✕)
132.77	604.85 ± 0.37	-0.14	77-orr/lau(✕)	190.72	535.82 ± 0.43	-0.32	77-orr/lau(✕)
138.35	598.34 ± 0.38	-0.33	77-orr/lau(✕)	194.57	530.80 ± 0.44	-0.39	77-orr/lau(✕)
140.65	595.78 ± 0.38	-0.27	77-orr/lau(✕)	199.01	524.91 ± 0.44	-0.48	77-orr/lau(✕)
143.72	592.31 ± 0.38	-0.23	77-orr/lau(✕)	203.19	519.47 ± 0.44	-0.36	77-orr/lau(✕)
146.45	589.12 ± 0.39	-0.29	77-orr/lau(✕)	207.43	513.49 ± 0.45	-0.60	77-orr/lau(✕)
149.05	586.22 ± 0.39	-0.19	77-orr/lau(✕)	212.62	506.27 ± 0.45	-0.63	77-orr/lau(✕)
151.91	582.94 ± 0.39	-0.16	77-orr/lau(✕)	218.53	497.97 ± 0.46	-0.52	77-orr/lau(✕)
154.66	579.78 ± 0.40	-0.13	77-orr/lau(✕)	222.94	491.64 ± 0.46	-0.39	77-orr/lau(✕)
157.49	576.68 ± 0.40	0.08	77-orr/lau(✕)	225.70	487.73 ± 0.47	-0.17	77-orr/lau(✕)
160.10	573.40 ± 0.40	-0.14	77-orr/lau(✕)	228.36	483.27 ± 0.47	-0.60	77-orr/lau(✕)
162.86	570.06 ± 0.40	-0.22	77-orr/lau(✕)	232.11	478.23 ± 0.47	0.17	77-orr/lau(✕)
165.65	566.71 ± 0.41	-0.26	77-orr/lau(✕)	90.35	651.92 ± 0.57	0.44	87-you/ely(✕)
168.64	563.23 ± 0.41	-0.17	77-orr/lau[1)]				

[1)] Not included in Fig. 1.

Further references: [14-maa/mci, 21-maa/wri, 38-kay, 41-lu/new, 62-mor, 64-cro/sco, 67-gil/zwi, 67-gue/ric, 68-klo/mck, 69-jen/kur, 70-tom-1, 71-chu/can, 71-str, 72-mil-1, 85-shi/gee].

Table 3. Recommended values (fit to the reliable experimental values according to the equations $\rho = A + BT + CT^2 + DT^3 + \ldots$ or $\rho = [1 + 1.75(1 - T/T_c)^{1/3} + 0.75(1 - T/T_c)][\rho_c + A(T_c - T) + B(T_c - T)^2 + C(T_c - T)^3 + D(T_c - T)^4]$).

$\frac{T}{K}$	$\frac{\rho \pm \sigma_{fit}}{kg \cdot m^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{fit}}{kg \cdot m^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{fit}}{kg \cdot m^{-3}}$
90.00	651.85 ± 0.48	170.00	561.77 ± 0.39	250.00	448.30 ± 0.25
100.00	641.19 ± 0.41	180.00	549.59 ± 0.40	260.00	429.52 ± 0.34
110.00	630.32 ± 0.39	190.00	537.06 ± 0.40	270.00	408.11 ± 0.32
120.00	619.29 ± 0.38	200.00	524.08 ± 0.40	280.00	382.92 ± 0.31
130.00	608.11 ± 0.37	210.00	510.55 ± 0.39	290.00	351.44 ± 0.31
140.00	596.79 ± 0.37	220.00	496.35 ± 0.37	293.15	339.25 ± 0.32
150.00	585.32 ± 0.38	230.00	481.34 ± 0.34	298.15	315.51 ± 0.36
160.00	573.65 ± 0.39	240.00	465.38 ± 0.30	300.00	304.30 ± 0.38

cont.

Ethane (cont.)

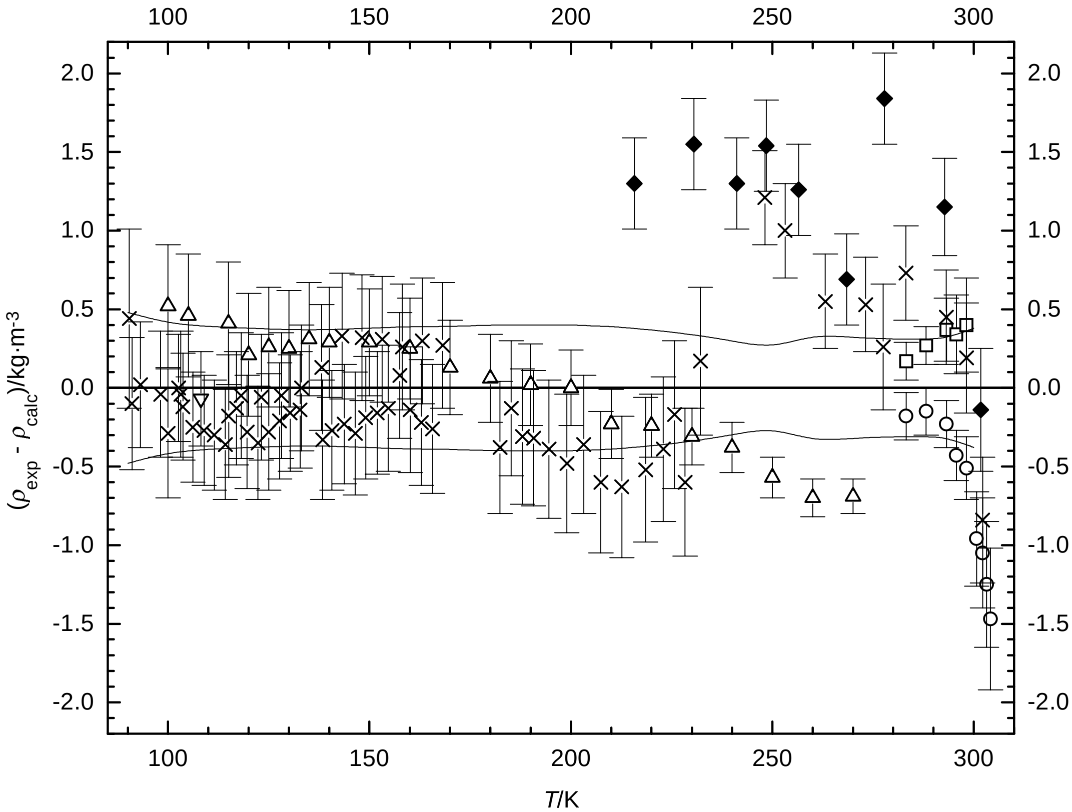


Fig. 1. The symbols show the deviation of the calculated from the experimental values from Table 2. The curves above and below the zero line indicate the calculated error region of the recommended values given in Table 3. The error bars are the experimental uncertainties. (Error bars smaller than the symbols are omitted to clarify the figure.)

Propane **[74-98-6]** **C_3H_8** **MW = 44.0965** **3**

T_c = 369.83 K [95-amb/tso]
ρ_c = 220.00 kg·m^{-3} [95-amb/tso]

Table 1. Coefficients for the polynomial expansion equations. Standard deviations (see introduction): $\sigma_\ell = 3.6824 \cdot 10^{-1}$ (low temperature range), $\sigma_{c,w} = 3.2514 \cdot 10^{-1}$ (combined temperature ranges, weighted), $\sigma_{c,uw} = 1.9543 \cdot 10^{-2}$ (combined temperature ranges, unweighted).

Coefficient	T = 85.47 to 288.00 K $\rho = A + BT + CT^2 + DT^3 + \ldots$	T = 288.00 to 369.83 K $\rho = [1 + 1.75(1 - T/T_c)^{1/3} + 0.75(1 - T/T_c)]$ $[\rho_c + A(T_c - T) + B(T_c - T)^2 + C(T_c - T)^3$ $+ D(T_c - T)^4]$
A	$8.20464 \cdot 10^{2}$	$4.90105 \cdot 10^{-1}$
B	-1.01300	$-1.32372 \cdot 10^{-2}$
C	$-2.71229 \cdot 10^{-4}$	$1.66441 \cdot 10^{-4}$
D	$3.32129 \cdot 10^{-6}$	$-7.65970 \cdot 10^{-7}$
E	$-1.12912 \cdot 10^{-8}$	

cont.

Propane (cont.)

Table 2. Experimental values with uncertainties and deviation from calculated values.

T/K	$\rho_{exp} \pm 2\sigma_{est}$ / $kg \cdot m^{-3}$	$\rho_{exp} - \rho_{calc}$ / $kg \cdot m^{-3}$	Ref. (Symbol in Fig. 1)	T/K	$\rho_{exp} \pm 2\sigma_{est}$ / $kg \cdot m^{-3}$	$\rho_{exp} - \rho_{calc}$ / $kg \cdot m^{-3}$	Ref. (Symbol in Fig. 1)
	crystal			214.15	599.80 ± 0.47	-0.16	63-see/urb[1)]
20.00	822.7 ± 7.7		30-heu[1)]	215.15	598.70 ± 0.47	-0.15	63-see/urb[1)]
20.00	809.1 ± 7.4		30-heu[1)]	216.15	597.70 ± 0.46	-0.03	63-see/urb[1)]
20.00	807.6 ± 7.4		30-heu[1)]	217.15	596.60 ± 0.46	-0.00	63-see/urb[1)]
77.00	763.0 ± 6.0		58-ste/lar[1)]	218.15	595.50 ± 0.46	0.02	63-see/urb[1)]
	liquid			219.15	594.40 ± 0.46	0.05	63-see/urb[1)]
230.71	582.20 ± 0.40	1.08	42-ano[1)]	220.15	593.20 ± 0.46	-0.02	63-see/urb[1)]
233.93	578.40 ± 0.40	1.04	42-ano[1)]	221.15	592.20 ± 0.45	0.11	63-see/urb[1)]
238.54	572.90 ± 0.40	0.99	42-ano[1)]	222.15	591.10 ± 0.45	0.15	63-see/urb[1)]
241.82	569.00 ± 0.40	1.00	42-ano(✕)	223.15	590.10 ± 0.45	0.28	63-see/urb[1)]
245.82	565.10 ± 0.40	1.93	42-ano[1)]	224.15	589.00 ± 0.45	0.33	63-see/urb[1)]
248.59	560.60 ± 0.40	0.82	42-ano(✕)	225.15	588.00 ± 0.45	0.47	63-see/urb[1)]
252.76	555.60 ± 0.40	0.96	42-ano(✕)	226.15	586.90 ± 0.44	0.52	63-see/urb[1)]
255.37	552.20 ± 0.40	0.82	42-ano(✕)	227.15	585.80 ± 0.44	0.57	63-see/urb[1)]
255.48	552.10 ± 0.40	0.86	42-ano(✕)	228.15	584.70 ± 0.44	0.62	63-see/urb[1)]
266.48	538.40 ± 0.45	1.23	42-ano[1)]	229.15	583.70 ± 0.44	0.78	63-see/urb[1)]
277.15	524.00 ± 0.45	1.04	42-ano[1)]	230.15	582.70 ± 0.44	0.93	63-see/urb[1)]
288.71	507.30 ± 0.50	0.43	42-ano[1)]	278.16	522.60 ± 0.27	1.01	63-see/urb[1)]
299.82	490.60 ± 0.50	0.82	42-ano[1)]	279.16	521.10 ± 0.27	0.88	63-see/urb[1)]
310.93	472.20 ± 0.50	1.24	42-ano[1)]	280.15	519.70 ± 0.27	0.84	63-see/urb[1)]
322.04	453.00 ± 0.55	2.45	42-ano[1)]	281.15	518.30 ± 0.27	0.82	63-see/urb[1)]
333.15	431.40 ± 0.55	3.64	42-ano[1)]	282.14	516.80 ± 0.27	0.69	63-see/urb[1)]
255.37	552.20 ± 0.40	0.82	42-car(✕)	283.14	515.30 ± 0.27	0.58	63-see/urb[1)]
266.48	538.40 ± 0.40	1.23	42-car[1)]	284.14	513.80 ± 0.27	0.47	63-see/urb[1)]
277.15	524.00 ± 0.40	1.04	42-car[1)]	285.15	512.40 ± 0.27	0.49	63-see/urb[1)]
288.71	507.30 ± 0.40	0.43	42-car[1)]	286.15	510.90 ± 0.28	0.40	63-see/urb[1)]
293.15	500.40 ± 0.40	0.11	42-car[1)]	287.16	509.40 ± 0.28	0.32	63-see/urb(∇)
299.82	490.60 ± 0.45	0.82	42-car[1)]	288.16	507.80 ± 0.28	0.14	63-see/urb[1)]
310.93	472.20 ± 0.45	1.24	42-car[1)]	289.16	506.30 ± 0.28	0.08	63-see/urb[1)]
322.04	453.00 ± 0.50	2.45	42-car[1)]	290.17	504.80 ± 0.28	0.05	63-see/urb[1)]
333.15	431.40 ± 0.55	3.64	42-car[1)]	291.12	503.30 ± 0.29	-0.04	63-see/urb[1)]
203.15	612.00 ± 0.49	-0.09	63-see/urb[1)]	292.15	501.70 ± 0.29	-0.10	63-see/urb[1)]
204.15	610.70 ± 0.49	-0.30	63-see/urb[1)]	293.15	500.14 ± 0.28	-0.15	63-see/urb[1)]
205.15	609.70 ± 0.49	-0.21	63-see/urb[1)]	293.15	500.15 ± 0.28	-0.14	63-see/urb[1)]
206.15	608.60 ± 0.48	-0.21	63-see/urb[1)]	294.14	498.60 ± 0.29	-0.17	63-see/urb[1)]
207.15	607.50 ± 0.48	-0.22	63-see/urb[1)]	295.14	497.00 ± 0.29	-0.23	63-see/urb[1)]
208.15	606.40 ± 0.48	-0.21	63-see/urb[1)]	295.15	497.00 ± 0.29	-0.21	63-see/urb[1)]
209.15	605.30 ± 0.48	-0.21	63-see/urb[1)]	296.15	495.50 ± 0.30	-0.15	63-see/urb[1)]
210.15	604.20 ± 0.48	-0.21	63-see/urb[1)]	297.15	493.90 ± 0.30	-0.17	63-see/urb[1)]
211.15	603.20 ± 0.47	-0.10	63-see/urb[1)]	297.21	493.80 ± 0.30	-0.17	63-see/urb[1)]
212.15	602.10 ± 0.47	-0.09	63-see/urb[1)]	298.18	492.20 ± 0.30	-0.22	63-see/urb[1)]
213.15	600.80 ± 0.47	-0.28	63-see/urb[1)]	299.18	490.60 ± 0.30	-0.22	63-see/urb[1)]

[1)] Not included in Fig. 1.

cont.

Propane (cont.)

Table 2. (cont.)

$\frac{T}{K}$	$\frac{\rho_{exp} \pm 2\sigma_{est}}{kg \cdot m^{-3}}$	$\frac{\rho_{exp} - \rho_{calc}}{kg \cdot m^{-3}}$	Ref. (Symbol in Fig. 1)	$\frac{T}{K}$	$\frac{\rho_{exp} \pm 2\sigma_{est}}{kg \cdot m^{-3}}$	$\frac{\rho_{exp} - \rho_{calc}}{kg \cdot m^{-3}}$	Ref. (Symbol in Fig. 1)
88.71	729.45 ± 0.33	-0.64	68-klo/mck(◆)	327.55	438.30 ± 0.40	-1.33	73-kah(✕)
94.26	724.07 ± 0.33	-0.39	68-klo/mck(◆)	93.15	725.36 ± 0.40	-0.22	76-mcc(✕)
99.82	718.62 ± 0.33	-0.21	68-klo/mck(◆)	98.15	720.31 ± 0.40	-0.21	76-mcc(✕)
105.37	712.95 ± 0.33	-0.26	68-klo/mck(◆)	103.15	715.20 ± 0.40	-0.25	76-mcc[1)]
110.93	707.39 ± 0.33	-0.19	68-klo/mck(◆)	108.15	710.08 ± 0.40	-0.31	76-mcc[1)]
116.48	701.76 ± 0.33	-0.20	68-klo/mck(◆)	113.15	704.98 ± 0.40	-0.35	76-mcc[1)]
122.04	696.16 ± 0.33	-0.17	68-klo/mck(◆)	118.15	699.98 ± 0.40	-0.29	76-mcc[1)]
127.59	690.43 ± 0.33	-0.28	68-klo/mck(◆)	123.15	694.92 ± 0.40	-0.29	76-mcc[1)]
133.15	684.81 ± 0.33	-0.26	68-klo/mck(◆)	128.15	689.76 ± 0.40	-0.38	76-mcc[1)]
283.20	514.30 ± 0.26	-0.34	69-sli[1)]	133.15	684.76 ± 0.40	-0.31	76-mcc[1)]
293.19	499.90 ± 0.26	-0.33	69-sli[1)]	138.15	679.82 ± 0.40	-0.17	76-mcc(✕)
303.15	484.30 ± 0.26	0.00	69-sli(✕)	143.15	674.69 ± 0.40	-0.21	76-mcc(✕)
313.12	467.44 ± 0.27	0.36	69-sli(✕)	148.15	669.60 ± 0.40	-0.20	76-mcc(✕)
323.12	448.73 ± 0.28	0.27	69-sli(✕)	153.15	664.52 ± 0.40	-0.16	76-mcc(✕)
333.11	428.20 ± 0.30	0.35	69-sli(✕)	158.15	659.50 ± 0.40	-0.05	76-mcc(✕)
343.08	403.78 ± 0.30	-0.04	69-sli(✕)	163.15	654.31 ± 0.40	-0.09	76-mcc(✕)
348.08	389.74 ± 0.30	0.07	69-sli(✕)	168.15	649.16 ± 0.40	-0.06	76-mcc(✕)
353.09	373.45 ± 0.30	0.13	69-sli(✕)	173.15	644.08 ± 0.40	0.06	76-mcc(✕)
358.10	353.75 ± 0.34	0.05	69-sli(✕)	100.07	719.06 ± 0.29	0.49	77-hay/hiz(Δ)
363.11	328.90 ± 0.46	0.64	69-sli(✕)	105.07	713.80 ± 0.29	0.29	77-hay/hiz(Δ)
368.10	286.10 ± 0.54	-0.11	69-sli(✕)	110.07	708.71 ± 0.28	0.26	77-hay/hiz(Δ)
369.10	268.10 ± 0.63	-0.95	69-sli(✕)	115.07	703.59 ± 0.28	0.20	77-hay/hiz(Δ)
369.60	250.00 ± 0.82	-3.09	69-sli[1)]	120.07	698.54 ± 0.28	0.21	77-hay/hiz(Δ)
278.15	521.90 ± 0.22	0.30	71-tom(○)	125.07	693.42 ± 0.28	0.16	77-hay/hiz(Δ)
283.15	515.00 ± 0.22	0.29	71-tom(○)	130.07	688.28 ± 0.28	0.09	77-hay/hiz(Δ)
288.15	507.70 ± 0.22	0.03	71-tom(○)	135.07	683.10 ± 0.27	-0.02	77-hay/hiz(Δ)
288.71	506.90 ± 0.22	0.03	71-tom(○)	140.07	677.99 ± 0.27	-0.04	77-hay/hiz(Δ)
293.15	500.30 ± 0.22	0.01	71-tom(○)	145.07	672.86 ± 0.27	-0.08	77-hay/hiz(Δ)
298.15	492.60 ± 0.24	0.13	71-tom(○)	150.07	667.62 ± 0.27	-0.21	77-hay/hiz(Δ)
303.15	484.60 ± 0.25	0.30	71-tom(○)	200.00	615.41 ± 0.25	-0.11	77-hay/hiz(Δ)
308.15	476.40 ± 0.26	0.59	71-tom(○)	240.00	570.04 ± 0.23	-0.13	77-hay/hiz(Δ)
313.15	467.80 ± 0.30	0.78	71-tom(○)	270.00	532.39 ± 0.21	-0.16	77-hay/hiz(Δ)
277.55	522.60 ± 0.40	0.18	73-kah[1)]	280.00	518.67 ± 0.21	-0.40	77-hay/hiz(Δ)
277.55	522.50 ± 0.40	0.08	73-kah[1)]	288.71	506.18 ± 0.20	-0.69	77-hay/hiz(Δ)
288.75	506.80 ± 0.40	-0.01	73-kah[1)]	86.65	732.24 ± 0.39	0.06	77-orr/lau(✕)
288.75	506.60 ± 0.40	-0.21	73-kah[1)]	90.10	728.50 ± 0.39	-0.18	77-orr/lau(✕)
299.86	490.00 ± 0.40	0.29	73-kah[1)]	96.04	722.44 ± 0.40	-0.22	77-orr/lau(✕)
299.86	489.80 ± 0.40	0.09	73-kah[1)]	100.98	717.47 ± 0.40	-0.18	77-orr/lau[1)]
310.95	471.70 ± 0.40	0.77	73-kah[1)]	106.17	712.18 ± 0.41	-0.22	77-orr/lau[1)]
310.95	471.60 ± 0.40	0.67	73-kah[1)]	111.51	706.72 ± 0.41	-0.27	77-orr/lau[1)]
327.55	438.40 ± 0.60	-1.23	73-kah[1)]	116.86	701.36 ± 0.42	-0.22	77-orr/lau[1)]

[1)] Not included in Fig. 1.

cont.

Propane (cont.)

Table 2. (cont.)

$\frac{T}{K}$	$\frac{\rho_{exp} \pm 2\sigma_{est}}{kg \cdot m^{-3}}$	$\frac{\rho_{exp} - \rho_{calc}}{kg \cdot m^{-3}}$	Ref. (Symbol in Fig. 1)	$\frac{T}{K}$	$\frac{\rho_{exp} \pm 2\sigma_{est}}{kg \cdot m^{-3}}$	$\frac{\rho_{exp} - \rho_{calc}}{kg \cdot m^{-3}}$	Ref. (Symbol in Fig. 1)
122.27	695.89 ± 0.42	-0.21	77-orr/lau[1)]	268.15	534.71 ± 0.16	-0.28	82-tho/har(□)
127.65	690.48 ± 0.43	-0.17	77-orr/lau[1)]	273.15	528.41 ± 0.16	0.05	82-tho/har(□)
133.13	684.82 ± 0.43	-0.27	77-orr/lau[1)]	278.15	521.62 ± 0.15	0.02	82-tho/har(□)
138.43	679.38 ± 0.44	-0.32	77-orr/lau[1)]	283.15	514.65 ± 0.17	-0.06	82-tho/har(□)
143.89	673.80 ± 0.44	-0.34	77-orr/lau(✕)	288.15	507.42 ± 0.17	-0.25	82-tho/har(□)
149.61	667.93 ± 0.45	-0.37	77-orr/lau(✕)	293.15	499.97 ± 0.17	-0.32	82-tho/har(□)
155.08	662.48 ± 0.46	-0.22	77-orr/lau(✕)	298.15	492.34 ± 0.18	-0.13	82-tho/har(□)
160.54	656.90 ± 0.46	-0.19	77-orr/lau(✕)	303.15	484.27 ± 0.18	-0.03	82-tho/har(□)
165.94	651.33 ± 0.47	-0.18	77-orr/lau(✕)	313.15	466.81 ± 0.18	-0.21	82-tho/har(□)
171.41	645.71 ± 0.47	-0.13	77-orr/lau(✕)	323.15	448.59 ± 0.19	0.19	82-tho/har(□)
182.34	634.26 ± 0.48	-0.13	77-orr/lau(✕)	333.15	427.60 ± 0.19	-0.16	82-tho/har(□)
187.80	628.48 ± 0.49	-0.13	77-orr/lau(✕)	343.15	403.22 ± 0.20	-0.41	82-tho/har(□)
193.30	622.60 ± 0.49	-0.14	77-orr/lau(✕)	348.15	389.15 ± 0.20	-0.30	82-tho/har(□)
198.89	616.65 ± 0.50	-0.07	77-orr/lau(✕)	353.15	373.01 ± 0.20	-0.10	82-tho/har(□)
204.54	610.55 ± 0.50	-0.03	77-orr/lau[1)]	358.15	353.65 ± 0.20	0.17	82-tho/har(□)
210.02	604.52 ± 0.51	-0.03	77-orr/lau[1)]	363.15	328.56 ± 0.24	0.54	82-tho/har(□)
216.02	597.85 ± 0.52	-0.02	77-orr/lau[1)]	365.15	315.11 ± 0.35	0.44	82-tho/har(□)
222.04	591.04 ± 0.52	-0.04	77-orr/lau[1)]	367.15	297.92 ± 0.46	0.58	82-tho/har(□)
227.36	584.99 ± 0.53	-0.00	77-orr/lau[1)]	368.15	286.01 ± 0.58	0.48	82-tho/har(□)
232.91	578.48 ± 0.53	-0.07	77-orr/lau[1)]	369.15	268.24 ± 0.81	0.37	82-tho/har[1)]
235.61	575.42 ± 0.54	0.04	77-orr/lau[1)]	244.67	564.86 ± 0.37	0.30	84-kra/mul(✕)
238.40	572.05 ± 0.54	-0.03	77-orr/lau[1)]	272.52	529.20 ± 0.36	-0.00	84-kra/mul[1)]
241.18	568.90 ± 0.54	0.14	77-orr/lau[1)]	284.52	512.64 ± 0.35	-0.15	84-kra/mul[1)]
243.98	565.63 ± 0.54	0.23	77-orr/lau[1)]	308.31	475.61 ± 0.34	0.07	84-kra/mul(✕)
258.15	547.46 ± 0.16	-0.42	82-tho/har(□)	324.56	445.82 ± 0.33	0.18	84-kra/mul(✕)
263.15	541.06 ± 0.16	-0.43	82-tho/har(□)	85.47	733.58 ± 0.37	0.21	87-you/ely(✕)

[1)] Not included in Fig. 1.

Further references: [21-maa/wri, 26-dan/jen, 34-sag/sch, 37-van, 40-des/bro, 43-cra-2, 55-cle/row-1, 62-mor, 68-sha/can, 69-jen/kur, 77-goo, 82-goo/hay, 71-str, 73-rod/mil].

Table 3. Recommended values (fit to the reliable experimental values according to the equations

$$\rho = A + BT + CT^2 + DT^3 + \dots \text{ or } \rho = [1 + 1.75(1 - T/T_c)^{1/3} + 0.75(1 - T/T_c)][\rho_c + A(T_c - T) + B(T_c - T)^2 + C(T_c - T)^3 + D(T_c - T)^4]\ ).$$

$\frac{T}{K}$	$\frac{\rho \pm \sigma_{fit}}{kg \cdot m^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{fit}}{kg \cdot m^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{fit}}{kg \cdot m^{-3}}$
	crystal	90.00	728.78 ± 0.36	140.00	678.10 ± 0.36
20.0	813	100.00	718.64 ± 0.34	150.00	667.91 ± 0.38
77.0	763	110.00	708.52 ± 0.34	160.00	657.65 ± 0.39
	liquid	120.00	698.40 ± 0.35	170.00	647.30 ± 0.41
80.00	738.93 ± 0.42	130.00	688.26 ± 0.35	180.00	636.85 ± 0.42

cont.

Propane (cont.)

Table 3. (cont.)

$\frac{T}{\mathrm{K}}$	$\frac{\rho \pm \sigma_{\mathrm{fit}}}{\mathrm{kg \cdot m^{-3}}}$	$\frac{T}{\mathrm{K}}$	$\frac{\rho \pm \sigma_{\mathrm{fit}}}{\mathrm{kg \cdot m^{-3}}}$	$\frac{T}{\mathrm{K}}$	$\frac{\rho \pm \sigma_{\mathrm{fit}}}{\mathrm{kg \cdot m^{-3}}}$
190.00	626.27 ± 0.43	260.00	545.53 ± 0.32	310.00	472.60 ± 0.31
200.00	615.52 ± 0.44	270.00	532.55 ± 0.26	320.00	454.44 ± 0.30
210.00	604.57 ± 0.44	280.00	519.07 ± 0.20	330.00	434.55 ± 0.29
220.00	593.39 ± 0.43	290.00	505.00 ± 0.26	340.00	411.74 ± 0.29
230.00	581.94 ± 0.41	293.15	500.29 ± 0.27	350.00	383.70 ± 0.30
240.00	570.17 ± 0.39	298.15	492.47 ± 0.29	360.00	344.97 ± 0.35
250.00	558.05 ± 0.36	300.00	489.49 ± 0.29		

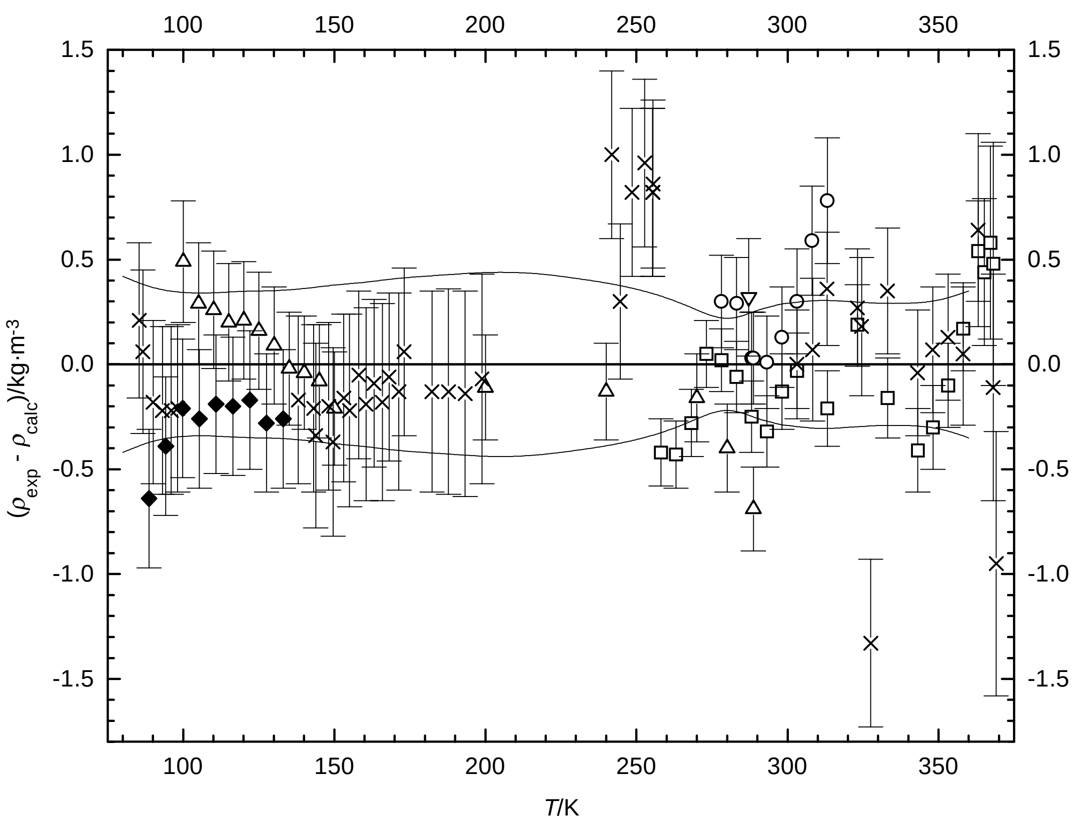


Fig. 1. The symbols show the deviation of the calculated from the experimental values from Table 2. The curves above and below the zero line indicate the calculated error region of the recommended values given in Table 3. The error bars are the experimental uncertainties. (Error bars smaller than the symbols are omitted to clarify the figure.)

Butane **[106-97-8]** **C_4H_{10}** **MW = 58.1234** **4**

T_c = 425.12 K [95-amb/tso]
ρ_c = 228.00 kg·m^{-3} [95-amb/tso]

cont.

Butane (cont.)

Table 1. Coefficients for the polynomial expansion equations. Standard deviations (see introduction): $\sigma_\ell = 3.9473 \cdot 10^{-1}$ (low temperature range), $\sigma_{c,w} = 3.3328 \cdot 10^{-1}$ (combined temperature ranges, weighted), $\sigma_{c,uw} = 6.9346 \cdot 10^{-2}$ (combined temperature ranges, unweighted).

Coefficient	T = 134.86 to 340.00 K $\rho = A + BT + CT^2 + DT^3 + \dots$	T = 340.00 to 425.12 K $\rho = [1 + 1.75(1 - T/T_c)^{1/3} + 0.75(1 - T/T_c)]$ $[\rho_c + A(T_c - T) + B(T_c - T)^2 + C(T_c - T)^3 + D(T_c - T)^4]$
A	$8.92907 \cdot 10^{2}$	$7.24403 \cdot 10^{-1}$
B	-1.45679	$-1.98517 \cdot 10^{-2}$
C	$2.87931 \cdot 10^{-3}$	$2.40924 \cdot 10^{-4}$
D	$-5.35281 \cdot 10^{-6}$	$-1.05134 \cdot 10^{-6}$

Table 2. Experimental values with uncertainties and deviation from calculated values.

$\frac{T}{\text{K}}$	$\frac{\rho_{exp} \pm 2\sigma_{est}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{exp} - \rho_{calc}}{\text{kg} \cdot \text{m}^{-3}}$	Ref. (Symbol in Fig. 1)	$\frac{T}{\text{K}}$	$\frac{\rho_{exp} \pm 2\sigma_{est}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{exp} - \rho_{calc}}{\text{kg} \cdot \text{m}^{-3}}$	Ref. (Symbol in Fig. 1)
	crystal			373.98	466.78 ± 0.49	1.39	40-kay-1(✕)
20.00	874.0 ± 6.6		30-heu	384.71	445.79 ± 0.54	0.83	40-kay-1(✕)
20.00	876.7 ± 6.6		30-heu	389.37	435.54 ± 0.56	0.39	40-kay-1(✕)
	liquid			393.76	425.13 ± 0.58	-0.01	40-kay-1(✕)
238.75	636.20 ± 0.44	-0.18	28-cof/maa[1)]	398.15	410.71 ± 0.61	-3.45	40-kay-1[1)]
240.35	634.60 ± 0.44	-0.18	28-cof/maa[1)]	402.04	404.47 ± 0.64	1.10	40-kay-1(✕)
242.95	631.80 ± 0.44	-0.37	28-cof/maa[1)]	405.87	391.17 ± 0.68	-0.32	40-kay-1(✕)
248.55	626.50 ± 0.43	-0.01	28-cof/maa[1)]	409.32	379.48 ± 0.72	0.08	40-kay-1(✕)
254.15	620.70 ± 0.43	-0.07	28-cof/maa[1)]	412.87	365.70 ± 0.78	0.61	40-kay-1(✕)
258.75	615.90 ± 0.43	-0.11	28-cof/maa[1)]	415.98	351.45 ± 0.85	1.10	40-kay-1(✕)
262.65	612.10 ± 0.43	0.18	28-cof/maa(✕)	419.26	333.82 ± 0.98	2.63	40-kay-1[1)]
266.45	608.10 ± 0.42	0.20	28-cof/maa[1)]	422.32	309.80 ± 1.24	3.38	40-kay-1[1)]
269.65	604.80 ± 0.42	0.31	28-cof/maa[1)]	213.15	661.60 ± 0.40	0.23	41-ben(✕)
272.35	602.00 ± 0.42	0.41	28-cof/maa[1)]	223.15	651.90 ± 0.40	0.18	41-ben(✕)
274.45	599.80 ± 0.42	0.49	28-cof/maa[1)]	233.15	642.10 ± 0.40	0.17	41-ben[1)]
281.65	592.80 ± 0.42	1.39	28-cof/maa[1)]	243.15	632.10 ± 0.40	0.13	41-ben[1)]
286.85	586.50 ± 0.41	0.90	28-cof/maa[1)]	253.15	622.00 ± 0.40	0.20	41-ben[1)]
288.65	584.40 ± 0.41	0.83	28-cof/maa[1)]	263.15	611.40 ± 0.40	0.00	41-ben(✕)
291.95	580.50 ± 0.41	0.69	28-cof/maa[1)]	273.15	600.80 ± 0.35	0.08	41-ben(✕)
296.45	575.30 ± 0.41	0.67	28-cof/maa[1)]	283.15	589.80 ± 0.35	0.05	41-ben[1)]
299.65	571.50 ± 0.41	0.61	28-cof/maa[1)]	293.15	578.70 ± 0.30	0.26	41-ben[1)]
302.45	568.10 ± 0.40	0.51	28-cof/maa[1)]	226.82	647.70 ± 0.25	-0.45	42-ano(○)
305.65	564.40 ± 0.40	0.62	28-cof/maa[1)]	235.87	638.90 ± 0.25	-0.34	42-ano(○)
325.04	541.10 ± 0.32	1.33	40-kay-1[1)]	238.65	636.00 ± 0.25	-0.48	42-ano(○)
336.48	525.73 ± 0.35	0.93	40-kay-1[1)]	247.76	627.20 ± 0.25	-0.11	42-ano(○)
345.65	513.07 ± 0.38	1.03	40-kay-1(✕)	255.37	619.70 ± 0.15	0.19	42-ano(○)
353.87	500.90 ± 0.41	1.50	40-kay-1(✕)	255.43	619.50 ± 0.15	0.05	42-ano(○)
361.21	489.04 ± 0.44	1.59	40-kay-1(✕)	266.48	608.20 ± 0.15	0.33	42-ano(○)
367.98	477.51 ± 0.46	1.54	40-kay-1(✕)	277.15	596.30 ± 0.15	-0.07	42-ano(○)

[1)] Not included in Fig. 1.

cont.

Butane (cont.)

Table 2. (cont.)

$\frac{T}{K}$	$\frac{\rho_{exp} \pm 2\sigma_{est}}{kg \cdot m^{-3}}$	$\frac{\rho_{exp} - \rho_{calc}}{kg \cdot m^{-3}}$	Ref. (Symbol in Fig. 1)	$\frac{T}{K}$	$\frac{\rho_{exp} \pm 2\sigma_{est}}{kg \cdot m^{-3}}$	$\frac{\rho_{exp} - \rho_{calc}}{kg \cdot m^{-3}}$	Ref. (Symbol in Fig. 1)
288.71	584.00 ± 0.15	0.50	42-ano(○)	160.07	711.92 ± 0.27	0.38	77-hay/hiz(Δ)
299.82	570.90 ± 0.15	0.21	42-ano(○)	165.07	706.98 ± 0.25	0.17	77-hay/hiz(Δ)
310.93	557.80 ± 0.15	0.39	42-ano(○)	170.07	702.36 ± 0.22	0.26	77-hay/hiz(Δ)
322.04	544.20 ± 0.15	0.60	42-ano(○)	230.00	644.65 ± 0.20	-0.38	77-hay/hiz(Δ)
333.15	529.40 ± 0.15	0.18	42-ano(○)	290.00	581.62 ± 0.14	-0.42	77-hay/hiz(Δ)
255.37	619.70 ± 0.40	0.19	42-car[1)]	300.00	570.21 ± 0.12	-0.27	77-hay/hiz(Δ)
266.48	608.20 ± 0.40	0.33	42-car(✕)	135.37	734.70 ± 0.34	-0.49	77-orr/lau(◆)
277.15	596.30 ± 0.40	-0.07	42-car[1)]	138.04	732.13 ± 0.35	-0.47	77-orr/lau(◆)
288.71	584.00 ± 0.40	0.50	42-car[1)]	139.44	730.88 ± 0.35	-0.36	77-orr/lau(◆)
299.82	570.90 ± 0.40	0.21	42-car[1)]	142.05	728.42 ± 0.35	-0.31	77-orr/lau(◆)
310.93	557.80 ± 0.40	0.39	42-car[1)]	144.78	725.91 ± 0.35	-0.19	77-orr/lau(◆)
322.93	544.20 ± 0.45	1.73	42-car[1)]	147.79	723.11 ± 0.36	-0.11	77-orr/lau(◆)
333.15	529.40 ± 0.45	0.18	42-car[1)]	150.53	720.55 ± 0.36	-0.05	77-orr/lau(◆)
310.93	557.16 ± 1.37	-0.25	44-old/rea[1)]	153.20	718.04 ± 0.36	-0.02	77-orr/lau(◆)
344.26	513.41 ± 1.19	-0.67	44-old/rea[1)]	155.93	715.48 ± 0.37	0.02	77-orr/lau(◆)
377.59	459.11 ± 0.97	0.34	44-old/rea(✕)	158.59	712.94 ± 0.37	-0.00	77-orr/lau(◆)
410.93	372.18 ± 0.69	-1.00	44-old/rea(✕)	161.37	710.35 ± 0.37	0.04	77-orr/lau(◆)
283.20	589.67 ± 0.07	-0.02	69-sli(□)	164.01	707.91 ± 0.37	0.10	77-orr/lau(◆)
293.20	578.28 ± 0.07	-0.10	69-sli(□)	166.65	705.49 ± 0.38	0.17	77-orr/lau(◆)
303.15	566.82 ± 0.07	0.06	69-sli(□)	169.52	702.81 ± 0.38	0.19	77-orr/lau(◆)
313.12	554.78 ± 0.08	0.05	69-sli(□)	172.20	700.24 ± 0.38	0.15	77-orr/lau(◆)
323.12	542.13 ± 0.08	-0.10	69-sli(□)	174.93	697.69 ± 0.38	0.16	77-orr/lau(◆)
333.11	529.06 ± 0.08	-0.22	69-sli(□)	177.71	695.10 ± 0.39	0.19	77-orr/lau(◆)
343.08	515.18 ± 0.09	-0.59	69-sli(□)	180.44	692.52 ± 0.39	0.18	77-orr/lau(◆)
353.09	500.24 ± 0.09	-0.40	69-sli(□)	183.50	689.57 ± 0.39	0.11	77-orr/lau(◆)
363.11	484.20 ± 0.10	-0.07	69-sli(□)	186.37	686.88 ± 0.40	0.12	77-orr/lau(◆)
368.10	475.82 ± 0.10	0.05	69-sli(□)	189.09	684.23 ± 0.40	0.03	77-orr/lau(◆)
288.75	584.40 ± 0.40	0.94	73-kah[1)]	191.79	681.66 ± 0.40	0.00	77-orr/lau(◆)
327.55	536.90 ± 0.40	0.36	73-kah(✕)	194.49	679.09 ± 0.40	-0.02	77-orr/lau(◆)
327.55	537.00 ± 0.40	0.46	73-kah(✕)	197.25	676.35 ± 0.41	-0.15	77-orr/lau(◆)
143.15	727.36 ± 0.40	-0.31	76-mcc(✕)	202.74	670.99 ± 0.41	-0.31	77-orr/lau(◆)
148.15	722.76 ± 0.40	-0.11	76-mcc[1)]	204.29	669.68 ± 0.41	-0.15	77-orr/lau(◆)
153.15	718.22 ± 0.40	0.11	76-mcc[1)]	205.43	668.61 ± 0.41	-0.13	77-orr/lau(◆)
158.15	713.53 ± 0.40	0.17	76-mcc[1)]	208.23	665.96 ± 0.42	-0.12	77-orr/lau(◆)
163.15	708.87 ± 0.40	0.24	76-mcc[1)]	211.02	663.23 ± 0.42	-0.18	77-orr/lau(◆)
168.15	704.26 ± 0.40	0.35	76-mcc(✕)	213.85	660.42 ± 0.42	-0.28	77-orr/lau(◆)
173.15	699.55 ± 0.40	0.35	76-mcc(✕)	216.62	657.86 ± 0.43	-0.18	77-orr/lau(◆)
135.07	735.36 ± 0.35	-0.12	77-hay/hiz(Δ)	219.35	655.14 ± 0.43	-0.26	77-orr/lau(◆)
140.07	730.65 ± 0.33	0.02	77-hay/hiz(Δ)	222.09	652.52 ± 0.43	-0.23	77-orr/lau(◆)
145.07	726.08 ± 0.32	0.26	77-hay/hiz(Δ)	224.97	649.46 ± 0.44	-0.49	77-orr/lau[1)]
150.07	721.25 ± 0.30	0.21	77-hay/hiz(Δ)	230.62	644.16 ± 0.44	-0.26	77-orr/lau[1)]
155.07	716.66 ± 0.28	0.38	77-hay/hiz(Δ)	233.39	641.35 ± 0.44	-0.34	77-orr/lau[1)]

[1)] Not included in Fig. 1.

cont.

Butane (cont.)

Table 2. (cont.)

$\frac{T}{K}$	$\frac{\rho_{exp} \pm 2\sigma_{est}}{kg \cdot m^{-3}}$	$\frac{\rho_{exp} - \rho_{calc}}{kg \cdot m^{-3}}$	Ref. (Symbol in Fig. 1)	$\frac{T}{K}$	$\frac{\rho_{exp} \pm 2\sigma_{est}}{kg \cdot m^{-3}}$	$\frac{\rho_{exp} - \rho_{calc}}{kg \cdot m^{-3}}$	Ref. (Symbol in Fig. 1)
236.11	638.64 ± 0.45	-0.36	77-orr/lau[1)]	220.00	653.61 ± 0.65	-1.16	89-vas/kha[1)]
241.56	633.07 ± 0.45	-0.50	77-orr/lau[1)]	230.00	644.81 ± 0.65	-0.22	89-vas/kha[1)]
244.34	630.28 ± 0.45	-0.49	77-orr/lau[1)]	240.00	634.89 ± 0.70	-0.24	89-vas/kha[1)]
247.21	627.35 ± 0.46	-0.52	77-orr/lau[1)]	250.00	624.80 ± 0.80	-0.23	89-vas/kha[1)]
249.97	624.47 ± 0.46	-0.59	77-orr/lau[1)]	260.00	614.51 ± 1.00	-0.19	89-vas/kha[1)]
252.25	622.06 ± 0.46	-0.67	77-orr/lau[1)]	270.00	603.98 ± 1.20	-0.14	89-vas/kha[1)]
255.36	618.94 ± 0.47	-0.58	77-orr/lau[1)]	280.00	593.17 ± 1.20	-0.07	89-vas/kha[1)]
258.25	615.95 ± 0.47	-0.58	77-orr/lau[1)]	290.00	582.04 ± 1.20	0.00	89-vas/kha[1)]
261.02	613.04 ± 0.47	-0.59	77-orr/lau[1)]	300.00	570.54 ± 1.20	0.06	89-vas/kha[1)]
263.79	610.09 ± 0.47	-0.63	77-orr/lau[1)]	310.00	558.61 ± 1.20	0.07	89-vas/kha[1)]
266.73	607.00 ± 0.48	-0.61	77-orr/lau[1)]	320.00	546.17 ± 1.20	-0.00	89-vas/kha[1)]
269.40	604.11 ± 0.48	-0.65	77-orr/lau[1)]	330.00	533.14 ± 1.20	-0.22	89-vas/kha[1)]
273.04	600.18 ± 0.48	-0.66	77-orr/lau[1)]	340.00	519.40 ± 2.00	-0.66	89-vas/kha[1)]
274.97	598.05 ± 0.49	-0.70	77-orr/lau[1)]	350.00	504.82 ± 2.00	-0.65	89-vas/kha[1)]
233.00	641.68 ± 0.35	-0.40	78-cal/mcl(∇)	360.00	489.18 ± 2.00	-0.28	89-vas/kha[1)]
134.86	735.26 ± 0.47	-0.42	87-you/ely(✕)	365.00	480.99 ± 2.00	-0.09	89-vas/kha[1)]
311.09	557.40 ± 0.40	0.19	89-nie[1)]	370.00	472.22 ± 2.00	-0.24	89-vas/kha[1)]
344.43	512.70 ± 0.70	-1.13	89-nie(✕)	375.00	463.12 ± 2.00	-0.42	89-vas/kha[1)]
394.60	422.20 ± 0.80	-0.92	89-nie(✕)	380.00	453.92 ± 2.00	-0.31	89-vas/kha(✕)
134.86	735.27 ± 0.74	-0.41	89-vas/kha[1)]	385.00	443.32 ± 2.00	-1.05	89-vas/kha(✕)
140.00	730.40 ± 0.73	-0.30	89-vas/kha[1)]	390.00	432.39 ± 2.00	-1.37	89-vas/kha(✕)
150.00	720.96 ± 0.72	-0.15	89-vas/kha[1)]	395.00	420.57 ± 2.00	-1.58	89-vas/kha[1)]
160.00	711.55 ± 0.71	-0.06	89-vas/kha[1)]	400.00	407.58 ± 2.00	-1.59	89-vas/kha(✕)
170.00	702.15 ± 0.70	-0.02	89-vas/kha[1)]	405.00	393.03 ± 2.00	-1.29	89-vas/kha(✕)
180.00	692.74 ± 0.69	-0.02	89-vas/kha[1)]	410.00	376.21 ± 2.00	-0.61	89-vas/kha[1)]
190.00	683.30 ± 0.68	-0.04	89-vas/kha[1)]	415.00	355.70 ± 2.00	0.43	89-vas/kha(✕)
200.00	673.81 ± 0.67	-0.09	89-vas/kha[1)]	420.00	327.65 ± 2.00	1.59	89-vas/kha(✕)
210.00	664.24 ± 0.66	-0.15	89-vas/kha[1)]	425.00	256.93 ± 2.00	2.61	89-vas/kha[1)]

[1)] Not included in Fig. 1.

Further references: [26-dan/jen, 37-sag/web, 40-kay, 43-cra-2, 49-foe/fen, 56-con, 56-hel/joe, 57-hel/ric, 67-gil/zwi, 80-tho/mil, 81-luo/mil, 82-hay/goo, 84-mas/hay].

Table 3. Recommended values (fit to the reliable experimental values according to the equations
$\rho = A + BT + CT^2 + DT^3 + \ldots$ or $\rho = [1 + 1.75(1 - T/T_c)^{1/3} + 0.75(1 - T/T_c)][\rho_c + A(T_c - T) + B(T_c - T)^2 + C(T_c - T)^3 + D(T_c - T)^4]$).

$\frac{T}{K}$	$\frac{\rho \pm \sigma_{fit}}{kg \cdot m^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{fit}}{kg \cdot m^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{fit}}{kg \cdot m^{-3}}$
	crystal	140.00	730.70 ± 0.34	180.00	692.76 ± 0.40
20.00	875.	150.00	721.11 ± 0.36	190.00	683.34 ± 0.39
	liquid	160.00	711.61 ± 0.38	200.00	673.90 ± 0.38
130.00	740.42 ± 0.32	170.00	702.17 ± 0.39	210.00	664.39 ± 0.37

cont.

Butane (cont.)

Table 3. (cont.)

$\frac{T}{K}$	$\frac{\rho \pm \sigma_{fit}}{kg \cdot m^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{fit}}{kg \cdot m^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{fit}}{kg \cdot m^{-3}}$
220.00	654.77 ± 0.35	293.15	578.44 ± 0.18	360.00	489.46 ± 0.30
230.00	645.03 ± 0.32	298.15	572.65 ± 0.18	370.00	472.46 ± 0.35
240.00	635.13 ± 0.30	300.00	570.48 ± 0.17	380.00	454.23 ± 0.44
250.00	625.03 ± 0.27	310.00	558.54 ± 0.17	390.00	433.76 ± 0.58
260.00	614.70 ± 0.25	320.00	546.17 ± 0.17	400.00	409.17 ± 0.82
270.00	604.12 ± 0.23	330.00	533.36 ± 0.18	410.00	376.82 ± 1.19
280.00	593.24 ± 0.20	340.00	520.06 ± 0.20	420.00	326.06 ± 1.65
290.00	582.04 ± 0.19	350.00	505.47 ± 0.26		

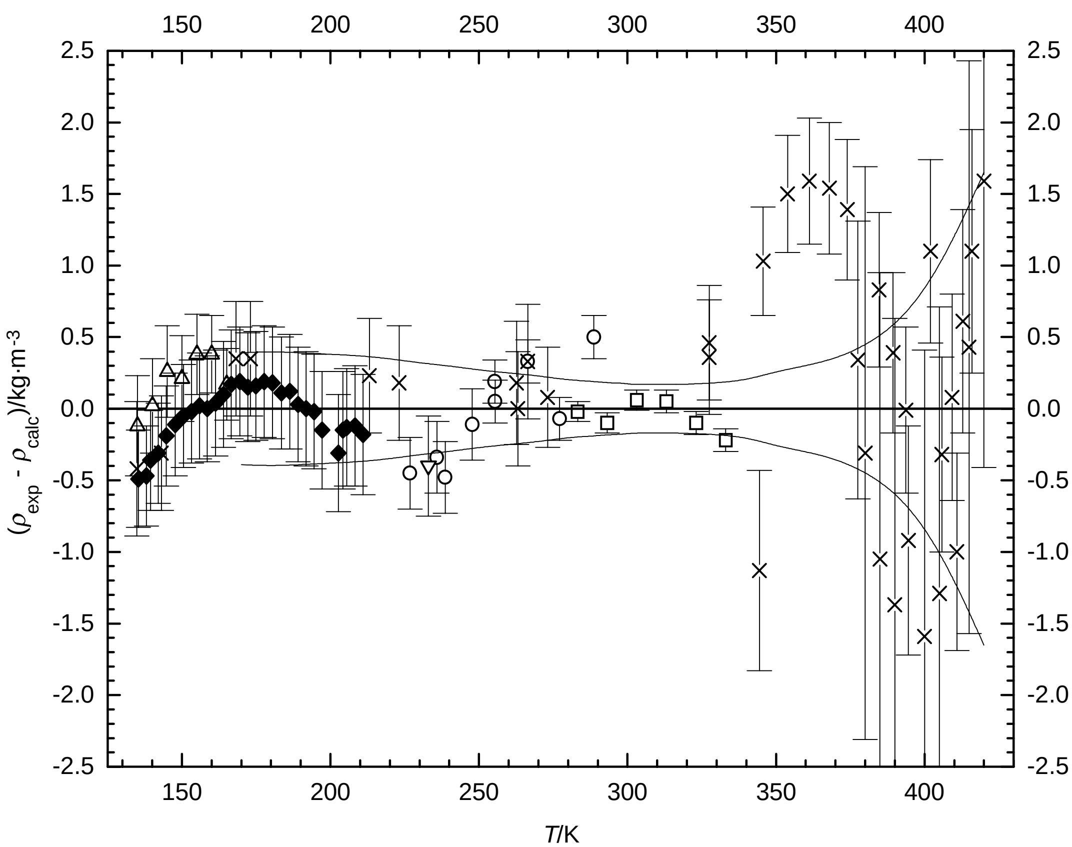


Fig. 1. The symbols show the deviation of the calculated from the experimental values from Table 2. The curves above and below the zero line indicate the calculated error region of the recommended values given in Table 3. The error bars are the experimental uncertainties. (Error bars smaller than the symbols are omitted to clarify the figure.)

Even Density, a so called simple property needs critical treatment

as was done by our authors and editors from TRC, now at NIST Boulder/Colorado

Graphical Presentation of the data with error bars for their uncertainties,

Temperature Dependence

Recommended values

Checking of Names, Determination and Drawing of standardized Structures, suitable for (sub)structure search