

# Physical Property Data Searching

Physical Property Compilations List - 2

## Sample Pages:

VNR INDEX OF CHEMICAL AND PHYSICAL DATA - 3

LANDOLT-BORNSTEIN - 4

FINDING PHYSICAL AND CHEMICAL PROPERTIES - 5

J. PHYSICAL & CHEMICAL REFERENCE DATA - 6-7

THERMOPHYS. PROPERTIES OF MATTER - 8-9

THERMOPHYS. PROPERTIES OF HIGH TEMP. SOLID MATERIALS - 10

THERMOPHYS. PROPERTIES RESEARCH LITERATURE...GUIDE - 11

EMIS DATAREVIEWS SERIES - 12

THERMODEX (Property Index to Thermodynamic Handbooks) - 13

THERMODYNAMIC DATA & PROPERTY CALCULATION WEB SITES - 14

knovel "ChemEssentials" Electronic Chemical References - 15

Polymer and Polymeric Materials Compilations - 16

Multivolume Compilations (Coordination, Organometallic, etc.) - 16

Spectra / Solubility Compilations - 17

Hazardous Property Data - 18

## Chemistry Library Web Page

Databases - Physical Properties

[library.caltech.edu/collections/chemistry.htm#DATABASESP](http://library.caltech.edu/collections/chemistry.htm#DATABASESP)

# PHYSICAL PROPERTY DATA SEARCHING

## CRC HANDBOOK OF CHEMISTRY AND PHYSICS

70<sup>th</sup> edition 1989-90, has deleted tables. Recent editions give data sources. MIL-8 QREF

## PERRY'S CHEMICAL ENGINEERS HANDBOOK / LANGE'S HANDBOOK ...

SFL REF TP151 .P45 1997 / SFL REF QD65 .L36 1999

## VNR INDEX OF CHEMICAL AND PHYSICAL DATA

Physical Property Tables, with literature references... MIL-8 QREF

## LANDOLT-BORNSTEIN, 6th ed. and New Series. ~200 v., 1950-1995

Comprehensive Data Compilation. MIL-8 / SFL REF QC61 L332

[http://link.springer.de/link/service/series/0284/tocs/000/start\\_0.pdf](http://link.springer.de/link/service/series/0284/tocs/000/start_0.pdf)

## FINDING PHYSICAL AND CHEMICAL PROPERTIES

<http://www.library.vanderbilt.edu/science/property.htm>

## J. PHYSICAL & CHEMICAL REFERENCE DATA - <http://ojps.aip.org/jpcrd/>

Physical Property and Spectral Data. Cumulative indexes 1-10,11-20,21-30

JPCRD SUPPLEMENTS / MONOGRAPHS (see CLAS)

e.g. Thermal Conductivity of the Elements, Atomic Transition Probabilities, etc.

## THERMOPHYS. PROPERTIES OF MATTER, v.1-14, 1970-79

Property/Temperature Diagrams. MIL-8 REF QC171 P83

## THERMOPHYS. PROPERTIES OF HIGH TEMP. SOLID MATERIALS, V.1-6, 1967

Materials with melting points above 800K or 1000F. MIL-8 REF TA418.26 P8

## THERMOPHYS. PROPERTIES RESEARCH LITERATURE...GUIDE, 1900-1980. 7v.

Separate 'chapter' for each physical property. MIL-8 REF Z5853.M38 T48 1982

## EMIS DATAREVIEWS SERIES

Databooks on semiconductors and other electronic materials.

Check CLAS for call numbers and locations

## THERMODEX (Property Index to Thermodynamic Handbooks)

<http://thermodex.lib.utexas.edu/>

## THERMODYNAMIC DATA & PROPERTY CALCULATION WEB SITES

[http://tigger.uic.edu/~mansoori/Thermodynamic.Data.and.Property\\_html](http://tigger.uic.edu/~mansoori/Thermodynamic.Data.and.Property_html)

## COMBINED CHEMICAL DICTIONARY (Range Searching)

<http://www.chemnetbase.com/scripts/ccdweb.exe>

# LANDOLT-BORNSTEIN

Comprehensive Physics, Chemistry, Astrophysics, Technical Data Collection

6<sup>th</sup> edition, 1950- (all volumes in German)

II/2a: Vapor Liquid Equilibria, Osmotic ...

II/2b-II/2c: Solution Equilibria

II/5a: Viscosity and Diffusion

NEW SERIES, 1961-

NS II/3: Luminescence of Organic Substances

NS II/5: Molecular Acoustics

NS II/13: Radical Reaction Rates in Liquids

NS II/16: Diamagnetic Susceptibilities

NS III/5: Structure Data of Organic Crystals

NS III/6: Structure Data of Elements ...

NS III/7: Crystal Structure Data of Inorganic ...

NS III/17: Semiconductors

NS III/26: Diffusion in Metals and Alloys

NS IV/1: Densities of Liquid Systems

NS IV/2: Heats of Mixing and Solution

NS IV/3: Thermodynamic Equilibria of Boiling ..

NS IV/4: High-Pressure Properties of Matter

NS V/1: Physical Properties of Rocks

NS VII: Crystallographic Data ... Nucleic Acids

INDEX: [http://link.springer.de/link/service/series/0284/tocs/000/start\\_0.pdf](http://link.springer.de/link/service/series/0284/tocs/000/start_0.pdf)

# Science and Engineering Library

## Finding Physical and Chemical Properties

<http://www.library.vanderbilt.edu/science/property.htm>

Activation Energies	Environmental Fate	Isoelectric Point
Activity Coefficients	Equilibrium Constants	Kinetic Data
Adsorption and Adsorption Coeff.	Expansion Coefficient	Lattice Energies
Antoine Coeff. and Constants	Explosive Properties	Log P
Atomic Mass Constant	Exposure Limits	Luminescence
Atomic Radius	Extinction Coefficient	Melting Point
Avogadro's Constant	Flammability	Molar Absorptivity
Bioconcentration Factor	Flash Point	Molecular Weight
Biodegradation	Free Energy	NFPA Chem. Hazard Label
Bohr Radius	Freezing Point	Octanol/H <sub>2</sub> O Partition
Boiling Point	Friction Coefficient	Optical Rotation
Boltzmann Constant	Fundamental Phys. Constants	Oxidn-Redn Potentials
Bond Energies	G-Factors	Oxidation States
Bond Lengths/Bond Angles	Gas Law	Ozone Depln Potential
Compressibility	Gibbs Free Energy	Partition Coefficients
Conductivity	Half Life	Phase Diagrams
Conversion factors	Hazard Ratings, Code/Rxns	Physical Properties
Corrosion	Heat Capacity	pK
Critical Properties	Heat of Combustion	Proton Affinity
Crystal Structure / Space Groups	Heat of Dilution	Radii
Debye-Huckel Coefficients	Heat of Formation	Rate Coefficients
Decomposition Rate	Heat of Fusion	Rate Constants
Degradation	Heat of Hydration	Refractive Index
Density	Heat of Ionization	Solubility
Dielectric Constant	Heat of Mixing	Space Groups
Diffusion (Molecular)	Heat of Neutralization	Specific Gravity
Dipole Moment	Heat of Polymerization	Specific Heat
Dissociation Constant	Heat of Reaction	Specific Rotation
Distribution Coefficient	Heat of Solution	Stability Constants
Electrical Conductivity	Heat of Sublimation	Surface Tension
Electrical Resistivity	Heat of Transformation	Tensile Strength
Electrode Potentials	Heat of Transition	Thermal Conductivity
Electron Affinity	Heat of Vaporization	Thermal Diffusivity
Electron Binding Energies	Henry's Law Constants, etc.	Thermal Expansion
Electron Configuration	Internuclear Distance	Thermodynamic Property
Electronegativity	Ionization Constant	Vapor Pressure
Enthalpy	Ionization Energy	Virial Coefficient
Enthalpy of	Ionization Heat	Viscosity
Entropy	Ionization Potential	Young's Modulus

Activation Energies

Handbook of antioxidants. 2nd ed.

Ref QD 281 O9 D45 2000

Polymer handbook. 4th ed.

Ref QD 388 .P65 1999

CRC handbook of bimolecular & termolecular gas reactions.

REF QD 502 .C18 1981-

## Journal of Physical and Chemical Reference Data. Monographs

1. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds
2. Gas-phase tropospheric chemistry of organic compounds
3. Vibrational and electronic energy levels of polyatomic transient molecules
4. Atlas of the vacuum ultraviolet emission spectrum of molecular hydrogen
5. Atlas of surface structures
6. Heat capacity of liquids : critical review and recommended values  
Heat capacity of liquids: supplement 1 (JPCRD 2001, 30(5),1199-1689)
7. Atomic transition probabilities of carbon, nitrogen, and oxygen
8. Spectral data for highly ionized atoms : Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Kr, and Mo
9. NIST-JANAF thermochemical tables

## Journal of Physical and Chemical Reference Data. Supplement ...

- v.2(1) Physical and thermodynamic properties of aliphatic alcohols
- v.3(1) Thermal conductivity of the elements
- v.6(1) Energetics of gaseous ions (ionization potentials, appearance potentials, and heats of formation of gaseous positive ions)
- v.10(1) Evaluated kinetic data for high temperature reactions, v.4  
Evaluated kinetic data ..., v.5, pt.1 (JPCRD 1986, 15(2),465-592)
- v.11(1) Thermophysical properties of fluids 1.  
Argon, ethylene, parahydrogen, nitrogen, nitrogen trifluoride, and oxygen
- v.11(2) NBS tables of chemical thermodynamic properties :  
selected values for inorganic & C1 & C2 organic substances in SI units
- v.13(1) Heat capacities and entropies of organic compounds in the condensed phase
- v.14(2) Atomic energy levels of the iron-period elements, potassium through nickel
- v.16(1) Atomic and ionic spectrum lines below 2000 angstroms : H2 thru Kr
- v.17(1) Gas-phase ion and neutral thermochemistry
- v.17(2) Thermodynamic and transport properties for molten salts :
- v.17(3) Atomic transition probabilities scandium through manganese
- v.17(4) Atomic transition probabilities iron through nickel

# EMIS datareviews series

1. Properties of Amorphous Silicon, 2nd. ed., 1989 (see v. 19)
2. Properties of Gallium Arsenide, 1st & 2nd. ed., 1986 & 1990 (see v. 16)
3. Properties of Mercury Cadmium Telluride, 1987
4. Properties of Silicon, 1988
5. Properties of Lithium Niobate, 1989 (see v. 28)
6. Properties of Indium Phosphide, 1991 (see v.21)
7. Properties of Aluminium Gallium Arsenide, 1993
8. Properties of Lattice-matched & Strained Indium Gallium Arsenide, 1993
9. Properties and Growth of Diamond, 1994 (see v. 26)
10. Properties of Narrow Gap Cadmium-based Compounds
11. Properties of Group III Nitrides, 1994
12. Properties of Strained and Relaxed Silicon Germanium, 1995
13. Properties of Silicon Carbide, 1995
14. Properties of Metal Silicides, 1995
15. Properties of III-V Quantum Wells and Superlattices, 1996
16. Properties of Gallium Arsenide, 3rd edition, 1996
17. Properties of Wide Bandgap II-VI Semiconductors, 1997
18. Properties of Porous Silicon, 1997
19. Properties of Amorphous Silicon and its Alloys, 1998
20. Properties of Crystalline Silicon, 1999
21. Properties, Processing and Applications of Indium Phosphide, 2000
22. Properties, Processing and Applications of Glass and Rare Earth-doped Glasses for Optical Fibres, 1998
23. Properties, Processing and Applications of Gallium Nitride and Related Semiconductors, 1999
24. Properties of Silicon Germanium and SiGe: carbon, 2000
25. Physical Properties of Liquid Crystals: nematics, 2001
26. Properties, Growth and Applications of Diamond, 2001
28. Properties of Lithium Niobate, new ed., 2002
29. Properties of Amorphous Carbon, 2003

# UIC Thermodynamics Research Laboratory

## Nano, Quantum & Statistical Mechanics & Thermodynamics

<http://tigger.uic.edu/~mansoori/Thermodynamic.Data.and.Property.html>

### Data & Property Calculation Websites

Acoustic Material Property Tables / SEA  
Atomic & Molecular Data in the NASA ADC Archives / CFA-Harvard  
Critical Temperatures and Pressures of Gases / Flexware  
Data for General, Organic, and Physical Chemistry: i.F & M College; ii.Colby College  
Data Search for Species by Chemical Formula / NIST  
Dielectric Constants / ASI Instruments Inc.  
Elemental Phase Diagrams of Many Binary and Some Ternary Mixtures / Georgia Tech  
F\*A\*C\*T (Facility for the Analysis of Chemical Thermodynamics) / École Poly. de Montréal  
Fundamental Constants / NIST  
Fundamental Physical Properties (MW; BP; critical constants; acentric factors)  
Heats of Combustion of Fuels / U Sydney  
Henry's Law Constants / Solubilities: Max Planck Inst.  
Ionization Energies, Electron Affinities and Electronegativities of the Elements / Tulane U  
Ionization Potentials / Electron Affinities / Munich Tech U  
Key values for standard enthalpy of formation and entropy at 298.15K / CODATA  
Metallurgical Thermodynamics Data & Software to download / NPL  
Mineralogy Database / webmineral.com  
Nanotechnology Database / Loyola U  
NIST WebBook: A gateway to the NIST data collection.  
Periodic Table of Elements and Their Properties: UBC/MIT/RXN Comm/Sheffield/Monachos  
Plastic Material Data Sheets / IDES  
Poly Ethylene Glycol Solution Properties: i.Densities; ii.Activity, Flory-Huggins X-  
Properties of 200 linear macromolecules and small molecules / ATHAS  
Refraction indices of some compounds / Conny  
RNA: Folding Free Energy & Enthalpy Tables / WUSTL  
Solubility Parameters on the Internet / Murdoch U  
Solvents Database / NCMS  
Sugar Engineer's Library -- Material Properties / sugartech.co  
Temperatures of Some Physical Phenomena / U Sydney  
Thermochemical databases (e.g. SGTE, geochemical) and data-files / GTT-Technologies  
Thermodynamic Properties of Minerals Databases / T.H. Brown  
ThermoDex: An Index of Selected Thermodynamic Data Handbooks / U Texas  
Third Millennium Thermodynamic Database for Combustion and Air-Pollution Use /Technion  
Validating Your Binary VLE Data / fortunecity.com

### Calculation / Program Download Sites

### Calculation / Program Request Sites

### Organizations Involved with Data Compilation and Property Calculation

### Bibliography:

# knovel "ChemEssentials" Electronic Chemical References

## [International Critical Tables of Numeric Data, Physics, Chemistry and Technology.](http://www.knovel.com/knovel2/Toc.jsp?BookID=735)

<http://www.knovel.com/knovel2/Toc.jsp?BookID=735>

*ICT* was originally published for the National Research Council, and offers physical, thermodynamic, mechanical, and other properties in chemistry, physics, and engineering. The *International Critical Tables* only contains seven interactive "knovelized" tables. This new process transforms tabular data to be Interactive Deep Searchable (IDS). IDS allows numeric searches by field and data manipulation in spreadsheet-like tables. The interactive 'knovelized' tables include:

Liquid Crystals - Table

Rotations and Melting Points of Pure Sugars and Sugar Derivatives - Table

Surface Tension Data for certain pure Liquids and Solutions ...- Table

Heats of Solution of Organic Substances - Table

The Electric Conductivity of Pure Non-Metallic Liquids - Table

Viscosity of Pure Liquids - Table

## [knovel Critical Tables \(academic edition\)](http://www.knovel.com/knovel2/Toc.jsp?BookID=761)

<http://www.knovel.com/knovel2/Toc.jsp?BookID=761>

*kCT* features tables of physical properties for commonly-used chemical compounds. *kCT* has expanded the original 6,000 chemical compounds in the physical properties tables of *International Critical Tables* to more than 13,000 compounds and contains the most up-to-date chemical properties information available online. Tables in *kCT* include:

Basic Physical Properties of Inorganic Compounds, ... Organic Compounds,

Critical Properties and Acentric Factor,

Enthalpy of Formation,

Enthalpy of Vaporization,

Entropy of Formation,

Entropy of Gas,

Gibbs Energy of Formation,

Heat Capacity of Gas,

Helmholtz Energy of Formation,

Internal Energy of Formation,

Basic Physical Properties ... Safety Properties of Common Solvents.

## [Thermochemistry of the Chemical Substances.](http://www.knovel.com/knovel2/Toc.jsp?BookID=744) (Rossini)

<http://www.knovel.com/knovel2/Toc.jsp?BookID=744>

This serves as a companion to the thermochemistry data in *International Critical Tables*. It includes 5,840 values of heats of formation and 350 values of heats of transition, fusion, vaporization, and reaction. All entries in the index are hyperlinked to their page numbers.

## [Smithsonian Physical Tables \(9th revised edition\).](http://www.knovel.com/knovel2/Toc.jsp?BookID=736)

<http://www.knovel.com/knovel2/Toc.jsp?BookID=736>

This reference comprises 901 tables concentrating on a broad scope of common physical and chemical data. On knovel, the *Smithsonian Physical Tables* are now easy to navigate and full text searchable (as are all references on knovel!). All entries in the index are hyperlinked to their page numbers.

# POLYMERS AND POLYMERIC MATERIALS

POLYMER HANDBOOK, 4th edition, 1999

Tabular data on polymerization, properties, nomenclature ... MIL-8 REF QD388 P65

POLYMER DATA HANDBOOK, 1999 <http://www.oup-usa.org/pdh/>

Key data on over two hundred polymers. SFL REF TA455 P58 P485

Encyclopedia of Polymer Science & Engineering, 2nd ed., v.1-18, 1985-1990

Physical and biological properties of polymers and plastics. MIL-8 REF TP1087 E46

<http://www.mrw.interscience.wiley.com/epst/index.html>

POLYMERIC MATERIALS ENCYCLOPEDIA, v.1-12, 1996

Synthesis, properties and applications of polymeric systems. MIL-8 REF TP1110 P65

CD-ROM available at SFL CIRC RESERVE TP1110 .P64 1996

COMPREHENSIVE POLYMER SCIENCE, v. 1-7, supp. 1-2, 1989-1996

Polymer Properties, Reactions, Processing and Specialty Polymers. MIL-8 REF QD381 C66

GE PLASTICS < [www.geplastics.com/](http://www.geplastics.com/) >

Resource for engineered thermoplastic resin materials

MATWEB <http://www.matweb.com/>

Information on over 30K materials including metals, plastics, ceramics, and composites.

RESIN SOURCE <http://ides.com/products/resinsource.asp?1>

Summary plastics data for 40K products from 390 global suppliers.

## Multivolume compilations:

Comprehensive Coordination Chemistry; Synthesis, reactions, properties & appl. v.1-7, 1987

Comprehensive Heterocyclic Chemistry; Structure, reactions, synthesis & uses. v.1-8, 1984

Comprehensive Heterocyclic Chemistry II. v.1-11, 1996 (literature – 1982-1995)

Comprehensive Medicinal Chemistry; Rational design, mechanistic ..., therapeutic appl. v.1-6, 1990

Comprehensive Natural Products Chemistry. v.1-9, 1999

Comprehensive Organic Chemistry; Synthesis & reactions. v.1-6, 1979

Comprehensive Organic Functional Group Transformations. v.1-7, 1995

Comprehensive Organic Synthesis; Selectivity, strategy, & efficiency ...v.1-9, 1991

Comprehensive Organometallic Chemistry; Synthesis, reactions, structures. v.1-9, 1982

Comprehensive Organometallic Chemistry II. v.1-14, 1995 (literature – 1982-1994)

Comprehensive Supramolecular Chemistry. v.1-11, 1996

Encyclopedia of Analytical Chemistry; Applications, theory and instrumentation. v.1-15, 2000

# SPECTRA / SOLUBILITY

SDBS <http://www.aist.go.jp/RIODB/SDBS/menu-e.html>

Integrated Spectral Data Base System for Organic Compounds (MS,NMR,IR, Raman, ESR)

SPECTRA ONLINE [http://spectra.galactic.com/SpectraOnline/Default\\_ie.htm](http://spectra.galactic.com/SpectraOnline/Default_ie.htm)

Public Domain FT-IR, UV-VIS, NIR, Raman, MS, NMR, XRD, etc.

MOLECULAR PROBES <http://www.probes.com/servlets/spectra/>

UV absorption and fluorescence emission spectra of commercial products

ALDRICH LIBRARY OF FT-IR SPECTRA, v.1-3, 1985

MIL-8 REF QD96 .I5 P66 1985

ALDRICH LIBRARY..13C & 1H FT NMR SPECTRA, v.1-3, 1993

MIL-8 REF QD96 .F68 P67 1993

FT-NIR ATLAS

MIL-8 REF QC462.85 .B83 1993

SADTLER .. IR (Inorganics & Organometallics)

MIL-8 REF QC453 .S23 & QC457 .S227

SIGMA LIBRARY ... FT-IR SPECTRA, v.1-2, 1986

MIL-8 REF QD96 .I5 K45 1986

UV ATLAS OF ORGANIC COMPOUNDS, v.1-5, 1966-71

MIL-8 REF QC459 .U85

ABSORPTION SPECTRA ... UV & VIS (LANG), v.1-24, 1966-1982 (indexes 1-5,6-10

Mil-8 REF QC437 .A19 (indexes 1-5,6-10,11-15,16-20)

HERSHENSON'S NMR / IR / UV INDEXES (lit. refs .. published spectra), ~1930-63

MIL-8 Quick Reference

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SOLUBILITIES (Stephen & Stephen), 7v. 1963-1979

Binary, Ternary and Multicomponent Systems

SOLUBILITIES (LINKE/SEIDELL), v.1-2, 1941-58

Organic, Inorganic and Metal-Organic Compounds

SOLUBILITY RESOURCES (CALTECH LIBRARY)

<http://library.caltech.edu/collections/rpb/chemistry/chemistrysupp.htm#Solubility%20Resources>

# HAZARDOUS PROPERTY DATA

TOXNET <http://www.nlm.nih.gov/pubs/factsheets/toxnetfs.html>

System of files related to toxicology, etc.

[HSDB \(HAZARDOUS SUBSTANCES DATABANK\)](#)

Extensive data on 4500 potentially hazardous chemicals. Fully referenced and peer-reviewed.

[CHEM IDplus](#)

Synonyms, CAS RNs, structures, regulatory information, and links to other databases.

[TOXLINE](#)

Bibliographic database (3M citations) focused on drugs and chemicals

[IRIS, CCRIS, GENE-TOX, DART/ETIC, TRI, NCI-3D](#)

ACUTE TOXICITY DATABASE <http://www.cerc.usgs.gov/data/acute/acute.html>

Compound/Species data (e.g. LC-50 data for various exposures)

ENVIRONMENTAL FATE DATA BASE

<http://esc.syrres.com/efdb.htm>

MATERIAL SAFETY DATA SHEETS

<http://www.ilpi.com/msds/index.html>

CALTECH CCE SAFETY MANUAL

<http://chemistry.caltech.edu/resources/safety.html>

CALTECH ENVIRONMENTAL HEALTH AND SAFETY OFFICE

<http://safety.caltech.edu/home.htm>

CHEM LIST - (Regulated Chemicals Listing) - (SciFinder Scholar)

227,000 Chemical Substances on ... Chemical Inventories and Regulatory Lists

Bretherick's HANDBOOK OF REACTIVE CHEMICAL HAZARDS, 6 ed., v.1-2, 1999

SFL REF T55.3.H3 B73

DANGEROUS PROPERTIES OF INDUSTRIAL MATERIALS (SAX), 6th ed., 1984

SFL REF / MIL-8 REF T55.3.H3 S3

SIGMA-ALDRICH LIBRARY OF CHEMICAL SAFETY DATA, v.1-2, 1988

MIL-8 REF T55.3.H3 S54

REGISTRY OF TOXIC EFFECTS OF CHEMICAL COMPOUNDS, V.1-5, 1985/86

SFL REF RA1215 .R4

DOSE (DICTIONARY OF SUBSTANCES AND THEIR EFFECTS, v.1-7, 1992-

SFL REF RA1193 .D53