

Sulfuric Acid

Other names:	Acide sulfurique Acido solforico BOV Battery acid Dihydrogen sulfate Dipping acid Electrolyte acid <chem>H2SO4</chem> HYDROGEN SULFATE Matting acid Mattling acid Nordhausen acid <chem>O2S(OH)2</chem> Oil of vitriol SULPHURIC ACID Schwefelsaeureloesungen Spirit of alum Spirit of vitriol Vitriol brown oil Vitriol, oil of Zwavelzuuroplossingen
Inchi:	<chem>InChI=1S/H2O4S/c1-5(2,3)4/h(H2,1,2,3,4)</chem>
InchiKey:	QAOWNCQODCNURD-UHFFFAOYSA-N
Formula:	<chem>H2O4S</chem>
SMILES:	<chem>O=S(=O)(O)O</chem>
Mol. weight [g/mol]:	98.08
CAS:	7664-93-9

Physical Properties

Property code	Value	Unit	Source
affp	699.40	kJ/mol	NIST Webbook
basg	683.00 ± 5.00	kJ/mol	NIST Webbook
basg	680.00	kJ/mol	NIST Webbook
basg	666.90	kJ/mol	NIST Webbook
ep	4.90	J/mol×K	NIST Webbook
gf	-793.06	kJ/mol	Joback Method

hf	-801.14	kJ/mol	Joback Method
hfpi	500.00 ± 20.00	kJ/mol	NIST Webbook
hfus	15.31	kJ/mol	Joback Method
hvap	67.59	kJ/mol	Joback Method
ie	12.40 ± 0.05	eV	NIST Webbook
log10ws	0.72		Crippen Method
logp	-0.653		Crippen Method
mcvol	50.690	ml/mol	McGowan Method
pc	12942.62	kPa	Joback Method
tb	431.54	K	Joback Method
tc	590.76	K	Joback Method
tf	249.96	K	Joback Method
vc	0.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	93.11	J/mol×K	431.54	Joback Method
cpg	95.72	J/mol×K	458.08	Joback Method
cpg	98.26	J/mol×K	484.61	Joback Method
cpg	100.73	J/mol×K	511.15	Joback Method
cpg	103.13	J/mol×K	537.68	Joback Method
cpg	105.43	J/mol×K	564.22	Joback Method
cpg	107.65	J/mol×K	590.76	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.70628e+01
Coeff. B	-6.85442e+03
Coeff. C	-5.92000e+01
Temperature range (K), min.	298.15
Temperature range (K), max.	610.00

Sources

- Comprehensive Thermochemical Study of Cyclic Five- and Six-Membered N-heterocycles using a rotating-bomb combustion calorimeter: Joback Method:**
- Thermochemistry of 1,3-diethylbarbituric and 1,3-dimethylbarbituric acids. Energetic study of benzothiazoles and two methylbenzothiazole derivatives by calorimetry and computation in $ZnSO_4 \cdot H_2O$, $MgSO_4 \cdot H_2SO_4 \cdot H_2O$ Systems at (30, 60, 90, and 120) kPa: combustion and enthalpies of formation of benzothiophene derivatives of barbituric acid and their derivatives: Crippen Method.**
- Densities and Viscosities of Niacin + 3-Picoline + Sulfuric Acid + Water from Electrical Conductivity of Electrolytes Found In Natural Waters from (5 to 90) Energetic and structural properties of 4-nitro-2,1,3-benzothiadiazole: Saturation Composition and Density Data for the Sodium Sulfate + Sulfuric Acid Yaws Handbook System Vapor Pressure: Freezing point depression in the ternary $ZnSO_4 \cdot H_2SO_4 \cdot H_2O$ system: Experimental study on the thermochemistry of 2-thiouracil, Standard enthalpies of formation of 2-aminothiophenothiazoles in the thermodynamic phase diagram of three thiophene carboxylic acid derivatives: Solubility of Sodium Naphthalene Disulfonate in Aqueous Solutions of Sulfuric Acid: 2-thiobarbituric and 2-thiobarbituric acids: An Crippen Method computational study: Thermochemical and thermophysical study of 2-thiophencarboxylic acid $MgSO_4 \cdot 7H_2O$ and 2-thiouracil in the $H_2O \cdot H_2SO_4 \cdot H_2O$ System at (30, 60, 90) and Temperature and Chemical Modeling of $MgSO_4 \cdot 7H_2O$ in the $H_2O \cdot H_2SO_4 \cdot H_2O$ System: key molecules: N-methylphenothiazine and The thermodynamics of Cu(II) and Ni(II) complexes with N-methylphenothiazine difference of sodium 4-nitrotoluene-2-sulfonate and determination of related systems: Preparation of 2,4-dinitrophenothiourea: Investigation of the preparation routes of benzotriazoles and the properties of Sulfuric Acid-Dimethylamine + Water Experimental and computational study on the energetics of Thermodynamic properties of naphthoxazole and naphthothiazole Knowledge: Experimental And Computational And Theoretical Study of the Structure and Entropy of substituted optical active phenylbenzazole Derivatives of p-Aminophenol Isole: Sulfuric acid + Water from (286.15 to 322.80) molality in 50 wt % H_2SO_4 at Elevated Temperatures and Pressures: McGowan Method:**
- Investigation of electrolytes of the vanadium redox flow battery (VII): Thermodynamic study of mixed $ZnCl_2$ - $VOSO_4$ solution ($VOSO_4 + H_2SO_4 + H_2O$) based on freezing-point depression and computational approaches:**
- <https://www.doi.org/10.1021/acs.jced.7b00083>
- <https://www.doi.org/10.1016/j.jct.2005.08.008>
- https://en.wikipedia.org/wiki/Joback_method
- <https://www.doi.org/10.1016/j.jct.2014.06.001>
- <https://www.doi.org/10.1016/j.jct.2013.06.021>
- <https://www.doi.org/10.1021/je5004252>
- <https://www.doi.org/10.1016/j.jct.2009.10.003>
- <https://www.doi.org/10.1016/j.jct.2019.01.014>
- <https://www.doi.org/10.1016/j.jct.2011.11.026>
- https://www.chemeo.com/doc/models/crippen_log10ws
- <https://www.doi.org/10.1021/je0496387>
- <https://www.doi.org/10.1021/je101012n>
- <https://www.doi.org/10.1016/j.jct.2012.01.018>
- <https://www.doi.org/10.1021/je049712l>
- <https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
- <https://www.doi.org/10.1016/j.jct.2018.12.043>
- <https://www.doi.org/10.1016/j.jct.2012.08.004>
- <https://www.doi.org/10.1016/j.jct.2014.01.018>
- <https://www.doi.org/10.1016/j.jct.2008.04.013>
- <https://www.doi.org/10.1021/je100020v>
- <https://www.doi.org/10.1016/j.tca.2015.12.007>
- <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
- <https://www.doi.org/10.1016/j.jct.2008.06.011>
- <https://www.doi.org/10.1021/je5010142>
- <https://www.doi.org/10.1021/acs.jced.5b01065>
- <https://www.doi.org/10.1016/j.jct.2015.10.013>
- <https://www.doi.org/10.1016/j.jct.2007.11.008>
- <https://www.doi.org/10.1016/j.fluid.2013.08.023>
- <https://www.doi.org/10.1016/j.fluid.2017.04.010>
- <https://www.doi.org/10.1021/je034225b>
- <https://www.doi.org/10.1016/j.jct.2013.08.026>
- <https://www.doi.org/10.1016/j.jct.2018.07.008>
- <https://www.doi.org/10.1021/je200549z>
- <https://www.doi.org/10.1016/j.jct.2017.08.017>
- <https://www.doi.org/10.1021/je049552d>
- <https://www.doi.org/10.1021/je4002366>
- <http://link.springer.com/article/10.1007/BF02311772>
- <https://www.doi.org/10.1016/j.jct.2019.02.020>
- <https://www.doi.org/10.1016/j.jct.2014.04.001>

Enthalpies of combustion and formation of 2-acetylpyrrole, 2-acetylphenylidene 2-acetylthiophene: 6-propyl-2-thiouracil: an experimental and computational study.	https://www.doi.org/10.1016/j.tca.2009.04.012
Experimental and computational thermochemical studies of 6-azauracil	https://www.doi.org/10.1016/j.jct.2015.12.020
Density and Viscosity of (4-Picoline + Water) Binary Mixtures from T = 298.15 K	https://www.doi.org/10.1021/acs.jced.5b00594
Experimental and computational study of the energetics of hydantoin and KDB	https://www.doi.org/10.1021/je8008182
KDB Hydantoin:	https://www.doi.org/10.1016/j.jct.2012.10.010
Thermochemistry of R-SH group in gaseous phase: Experimental and computational energies and formation enthalpies of 2-SH benzazoles:	https://www.doi.org/10.1016/j.mol.2016.09.001
Thermochemistry of substituted thiophenecarbonitrile derivatives: Measurement and correlation for the solubility of	https://www.doi.org/10.1016/j.fluid.2015.07.041
2,4-dihydro-4-sulfonic acid Nitrobenzene-Inorganic Acid Systems containing dibenzothiophene	https://www.doi.org/10.1021/je800878b
thermochemical data: Experimental and computational studies:	https://www.doi.org/10.1016/j.jct.2009.05.019
Thermophysical Properties of a 2,4,6,7-tetrathia Diazepine: Study of its structure, energetics and aromaticity: Calorimetric study of methyl and ethyl 2-thiophenecarboxylates and ethyl 2-NIST Webbook:	https://www.doi.org/10.1021/acs.jced.8b00466
Solubilities of Isonicotinic Acid in Sulfuric Acid + Water and	https://www.doi.org/10.1016/j.jct.2012.02.005
possible precursors and products of deep hydrodesulfurization in gasoline and distillates in n-heptane:	https://www.doi.org/10.1016/j.jct.2009.03.007
Creation, Ramplike Generation of	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7664939&Units=SI
Conformation and Vibrational	https://www.doi.org/10.1021/je900871q
Calorimetry of Phenol in Sulfuric Acid + Water	https://www.doi.org/10.1016/j.jct.2003.12.012
Standard enthalpies of formation	https://www.doi.org/10.1021/je1009366
and of sublimation of	https://www.doi.org/10.1021/je050443o
Thiophenecarboxylic Acid Surface	https://www.doi.org/10.1016/j.jct.2007.07.004
Tension of liquid-phase Beckmann Rearrangements Mixtures	https://www.doi.org/10.1021/je500836b
Computational study of benzofuran,	https://www.doi.org/10.1016/j.jct.2016.02.008
2-nitro-2H-pyran-4-one and their derivatives:	https://www.doi.org/10.1016/j.jct.2013.11.013
properties of phenoxazine and	https://www.doi.org/10.1016/j.jct.2018.11.001
perchlorate: dependence of the temperature	https://www.doi.org/10.1016/j.jct.2006.07.007
dependence of Titanium(IV) hydrolysis	https://www.doi.org/10.1016/j.jct.2012.09.007
Enthalpies of formation of two	https://www.doi.org/10.1016/j.jct.2016.07.006
bis(N,N-diethylthiocarbamoyl)hydric	
Solutions:	
Experimental redetermination of the	
gas-phase enthalpy of formation of	
FeSO4·7H2O	
Determination and chemical modeling	
of the solubility of FeSO4·7H2O in the	
Ti(SO4)2-H2SO4-H2O system:	

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
ep:	Protonation entropy at 298K
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfpi:	Enthalpy of formation of positive ion at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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