

Sulfuric Acid

Other names:	Acide sulfurique Acido solforico BOV Battery acid Dihydrogen sulfate Dipping acid Electrolyte acid H2SO4 HYDROGEN SULFATE Matting acid Mattling acid Nordhausen acid O2S(OH)2 Oil of vitriol SULPHURIC ACID Schwefelsaeureloesungen Spirit of alum Spirit of vitriol Vitriol brown oil Vitriol, oil of Zwavelzuuroplossingen
Inchi:	InChI=1S/H2O4S/c1-5(2,3)4/h(H2,1,2,3,4)
InchiKey:	QAOWNCQODCNURD-UHFFFAOYSA-N
Formula:	H2O4S
SMILES:	O=S(=O)(O)O
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		m ³ /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

- Thermodynamic properties of epsilon-caprolactam and possible applications: H₂SO₄ at Elevated Temperatures and Pressures: Liquid-Liquid Equilibria of Nitrobenzene-Inorganic Acid Systems
<https://www.doi.org/10.1016/j.jct.2019.01.014>
- Combustion energies and formation enthalpies of 2-SH-benzazoles: Experimental and computational thermochemical studies of 6-azauracil and of sublimation of 2-thiouracil
<https://www.doi.org/10.1021/je4002366>
- Review and analysis of the thermophysical properties of a Sulfuric Acid-Water Electrolyte:
<https://www.doi.org/10.1021/je800878b>
- Redesigning the rotating-bomb combustion calorimeter: Investigation of electrolytes of the vanadium redox flow battery (VII):
<https://www.doi.org/10.1016/j.jct.2008.02.018>
- Prohibition of combustion of mixed bis(N,N-dialkylammonium)SO₄ + H₂O based on Pyrom's theory of deep hydrodesulfurization of gasoline
<https://www.doi.org/10.1016/j.jct.2015.12.020>
- Thermodynamic properties of Ni(II) complexes with properties of N-acetylserine and N-acetylglutamate
<https://www.doi.org/10.1016/j.jct.2007.07.004>
- Study of cyclic Five- and Six-Membered Nucleosides and Nucleotides
<https://www.doi.org/10.1021/acs.jced.8b00466>
- 3-Picoline + Sulfuric Acid + Water from (298.15 to 373.15) K
<http://link.springer.com/article/10.1007/BF02311772>
- Determination of the energies of combustion and enthalpies of formation of the pyridine derivatives: Electrical Conductivity of Electrolytes Found In Natural Waters from (5 to 90) °C
<https://www.doi.org/10.1016/j.jct.2005.08.008>
- Phase Equilibria for the KHSO₄ H₂O and KHSO₄ CrO₃ H₂O Systems
<https://www.doi.org/10.1016/j.jct.2019.02.020>
- Formation of 2-acetylpyrrole, 2-thiouracil and the temperature dependence of Titanium(IV) hydrolysis
<https://www.doi.org/10.1016/j.jct.2006.07.007>
- Van der Waals Equilibria of the FeSO₄ H₂O System at (30, 50, 70, 90, 110, 130) kPa:
<https://www.doi.org/10.1016/j.jct.2003.12.012>
- Solubility Measurement and Chemical Modeling of MgSO₄*7H₂O in the Temperature Range 273-323 K:
<https://www.doi.org/10.1016/j.jct.2007.11.008>
- Resolving the thermodynamic thermochemical data: Experimental and computational study of the thermodynamics of substituted thiophenecarbonitrile derivatives: Determination of related systems' solubility data (I) in the preparation process of K₂SO₄ or KH₂PO₄ by the solvent extraction method:
<https://www.doi.org/10.1021/acs.jced.7b00083>
- Experimental study on the thermochemistry of 2-thiouracil, 5-henopyridin-2(1H)-one and 2-thiobarbituric acids: An experimental study on the thermodynamic properties of N-methylphenothiazine and N-methylisocytizine
<https://www.doi.org/10.1021/je0496387>
- Tension of Liquid Phase Beckmann Rearrangement: Thermophysical study of 2-thiophenecarboxylic acid
<https://www.doi.org/10.1016/j.jct.2009.10.003>
- Standard enthalpies of formation of 2-phenylbenzothiazoles in the presence of NaClO₄ (aq) + H₂O (l) Binary Mixtures from T (298.15 to 373.15) K
<https://www.doi.org/10.1016/j.jct.2008.04.013>
- Thermodynamics of 6-propyl-2-thiouracil: an experimental determination of the gas-phase enthalpy of formation of 2-thiouracil
<https://www.doi.org/10.1021/je101012n>
- Solubility of Isonicotinic Acid in Sulfuric Acid + Water and 4-Methylpyridine + Sulfuric Acid + Water from (293.55 to 361.45) K:
<https://www.doi.org/10.1021/acs.jced.5b00594>
- <https://www.doi.org/10.1016/j.jct.2009.04.012>
- <https://www.doi.org/10.1016/j.jct.2018.11.001>
- <https://www.doi.org/10.1021/je5010142>
- https://www.chemeo.com/doc/models/crippen_log10ws
- <https://www.doi.org/10.1021/acs.jced.5b01065>
- <https://www.doi.org/10.1016/j.jct.2009.05.019>
- <https://www.doi.org/10.1021/je100020v>
- <https://www.doi.org/10.1016/j.jct.2007.06.020>
- <https://www.doi.org/10.1016/j.fluid.2017.04.010>
- <http://webbook.nist.gov/cgi/cbook.cgi?ID=C7664939&Units=SI>
- <https://www.doi.org/10.1016/j.jct.2012.08.004>
- <https://www.doi.org/10.1016/j.tca.2015.12.007>
- <https://www.doi.org/10.1016/j.jct.2015.10.013>
- <https://www.doi.org/10.1021/je500836b>
- <https://www.doi.org/10.1016/j.jct.2008.06.011>
- <https://www.doi.org/10.1016/j.jct.2014.01.018>
- <https://www.doi.org/10.1021/je8008182>
- <https://www.doi.org/10.1016/j.tca.2014.04.018>
- <https://www.doi.org/10.1016/j.jct.2012.09.007>
- <https://www.doi.org/10.1021/je900871q>

Thermochemistry of 1,3-diethylbarbituric acid: the experimental and computational study: the laws of the perfect gas: Vapor pressure: https://www.doi.org/10.1016/j.jct.2014.06.001

Measurement and correlation for the solubility of 2-chloro-5-hydroxybenzoic acid: https://www.doi.org/10.1016/j.fluid.2015.07.041

Experimental and computational study of the energetics of hydantoin and its zwitterion: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

2-amino-3-chloro-4-methylbenzenesulfonic acid: https://www.doi.org/10.1016/j.jct.2012.10.010

2-aminothiazole and computational study on the energetics of five five-membered benzothiazole and two methylbenzothiazole derivatives: https://www.doi.org/10.1016/j.jct.2013.08.026

Determination and chemical modeling of the solubility of $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$ in the $\text{H}_2\text{SO}_4\text{-H}_2\text{O}$ system: reactivity properties of phenoxazine and phenothiazine: https://www.doi.org/10.1016/j.jct.2013.06.021

Thermodynamic study of 2-aminothiazole and 2-amino-3-chloro-4-methylbenzenesulfonic acid: https://www.doi.org/10.1016/j.jct.2016.07.006

Amidic and thiazole properties of 4-nitro-2,3-dimethylthiadiazoles: https://www.doi.org/10.1016/j.jct.2013.11.013

Vapor Liquid Equilibria for the $\text{ZnSO}_4\text{-H}_2\text{SO}_4\text{-H}_2\text{O}$ and $\text{MgSO}_4\text{-H}_2\text{SO}_4\text{-H}_2\text{O}$ systems: https://www.doi.org/10.1016/j.jct.2014.04.001

Synthesis, structure, conformational analysis of 2-thiophenecarboxylates and ethyl 2-sulfur-containing ionic Liquids. https://www.doi.org/10.1016/j.jct.2012.01.018

Rotating-Bomb Combustion Calorimetry and Reaction Principles: https://www.doi.org/10.1021/je5004252

Formation of benzenesulfonamide and sulfuric acid: https://www.doi.org/10.1016/j.jct.2009.03.007

Sulfuric Acid + Dimethylamine + Water Solutions of a Molecule: An Experimental and Theoretical Study of the Structure and Enthalpy of Formation of Tetrahydro-2H-1,3-oxazine-2-thione: https://www.doi.org/10.1021/je1009366

Experimental and computational thermochemical study of benzofuran, benzimidazole and its derivatives: https://www.doi.org/10.1016/j.jct.2011.11.026

ternary $\text{ZnSO}_4\text{-H}_2\text{SO}_4\text{-H}_2\text{O}$ system: https://www.doi.org/10.1021/je034225b

2,1,3-Benzothiadiazole: study of its structure, energetics and aromaticity: KDB: https://www.doi.org/10.1021/je200549z

Thermodynamic properties of naphthoxazole and naphthothiazole derivatives: https://www.doi.org/10.1016/j.jct.2018.12.043

Experimental and Density Data for the Sodium Sulfate + Sulfuric Acid + Water System: https://www.doi.org/10.1016/j.jct.2012.02.005

Relative Henry's Law Constant of Phenol in Sulfuric acid + Water from (286.15 to 323.15) K: https://www.doi.org/10.1016/j.jct.2018.07.008

The thermochemistry of R-SH group in gaseous phase: Experimental and theoretical studies of the enthalpies and entropies of sulfur containing species in Sulfuric Acid + Water systems: https://www.doi.org/10.1021/je049712l

Thermodynamic and conformational study of optical active phenylbenzazole derivatives: https://www.doi.org/10.1021/je049552d

solubility of sodium 4-nitrotoluene-2-sulfonate and 4-nitrotoluene-2-sulfonic acid in (sulfuric acid + water) system: https://www.doi.org/10.1016/j.jct.2018.03.002

https://www.doi.org/10.1021/je050443o

https://www.doi.org/10.1016/j.jct.2017.08.017

https://www.doi.org/10.1016/j.fluid.2013.08.023

Legend

afp:	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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