

# 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	680.00	kJ/mol	NIST Webbook
basg	666.90	kJ/mol	NIST Webbook
basg	683.00 ± 5.00	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  
Heteromolecules; determination of the  
gas-phase enthalpy of formation of  
epsilon-caprolactam and  
benzothiazole derivatives;  
thermochemical data: Experimental  
and computational studies  
Pressure:  
Determination of the energies of  
combustion and enthalpies of  
formation of nitriles and amides  
Liquid Phase Beckmann  
Rearrangement Mixtures: bomb  
combustion calorimeter:  
Energetic study of benzothiazole and  
two methylbenzothiazole derivatives:  
Experimental and computational  
thermochemical studies of 6-azauracil  
derivatives  
solubility of  $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$  in the  
 $\text{H}_2\text{SO}_4$ - $\text{H}_2\text{O}$  mixtures and reactivity  
properties of phenoxazine and  
phenothiazine  
enthalpies of combustion of two  
bis(N,N-diethylthioureas):  
Investigation of electrolytes of the  
vanadium redox flow battery (VII):  
Polarographic Method  
electrolyte solution ( $\text{VOSO}_4 + \text{H}_2\text{SO}_4 +$   
 $\text{H}_2\text{O}$ ) based on Eyring's theory:

# Review and Analysis of Thermophysical Properties of a Investigation on the Solubility Difference of sodium 4-nitrotoluene-2-sulfonate and Experimental and Computational study on the energetic (e<sup>-</sup>) system: Nadeen M. Elshoridey

Energetic and structural properties of  
 4-nitro-2,1,3-benzothiadiazole:  
 5-Isopropylbarbituric and  
 2-thiobarbituric acids: An  
 Vapor-Liquid Equilibrium for the  $\text{ZnSO}_4$ -  
 experimental and computational study:  
 $\text{H}_2\text{SO}_4$ - $\text{H}_2\text{O}$  and  $\text{MgSO}_4$ - $\text{H}_2\text{SO}_4$ - $\text{H}_2\text{O}$   
 Systems at 0.1, 0.01, and 0.0013 kPa:  
 Experimental and Theoretical Study of  
 the Mechanism of the Substituted  
 thiobarbituric derivatives:  
 McGowan Method: oxazine-2-thione:

### Density and Viscosity of (4-Picoline + Water) Binary Mixtures from T<sub>1</sub> (298.15 to 338.05 K)

Complexes with  
Experimental Study of the Phenylthiourea  
Thermochemistry of 2-thiouracil,  
Kinetic and Thermodynamic Parameters of  
Sintering of Optical Active Phenylbenzazole  
Depression in  
the ternary ZnSO<sub>4</sub>-H<sub>2</sub>SO<sub>4</sub>-H<sub>2</sub>O system:  
Thermochemistry of R-SH group in  
gaseous phase: Experimental and  
Theoretical studies of related systems'  
Solubility data drive the preparation  
process of MgSO<sub>4</sub> from H<sub>2</sub>O by the  
Modeling of MgSO<sub>4</sub>-H<sub>2</sub>O in the  
FeSO<sub>4</sub>-H<sub>2</sub>SO<sub>4</sub>-H<sub>2</sub>O System: formation  
and of sublimation of  
Enthalpies of combustion and  
formation of 2-acetylpyrrole,  
2-azetidine and 2-furanone.  
Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> H<sub>2</sub>SO<sub>4</sub>-H<sub>2</sub>O System at (30,  
0.55) and (0.69, 0.3) kPa:

### Thermochemical properties of three 2-thiophenecarboxylic acid derivatives:

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[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

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KDB:

Energetic insights on two dye key molecules: N-methylphenothiazine and 1-methylphenothiazine:  
Thermodynamics of:  
6-propyl-2-thiouracil: an experimental and computational study  
Sodium Naphthalene Disulfonate in Aqueous Solutions of 2,1,4-Benzothiadiazole: study of its structure, energetics and aromaticity: Measurement and correlation for the solubility of  
Electro-Conductivity of Electrolytes and Found In Natural Waters from (5 to 90) °C  
The 5-(1,1,1,4-tetramethylbenzenesulfonic acid) and 5-(1,1,1,4-tetramethylbenzenesulfonic acid) derivatives:  
Sulfuric acid + Water from (286.15 to 323.15) K: Determination of the temperature dependence of Titanium(IV) hydrolysis and sulfuric acid concentration in Sulfuric Acid + Water and hydrolytic reactions of sulfuric acid and ethyl phenylphosphonate and ethyl 2- and 3-aminobenzoates of p-Aminophenol in Sulfuric Acid + Water at temperatures from (293.15 to 343.15) K  
3,3-diethylbarbituric and Phase Equilibria for the  $\text{H}_2\text{SO}_4$ - $\text{H}_2\text{SO}_4$ - $\text{H}_2\text{O}$  and  $\text{H}_2\text{SO}_4$ - $\text{H}_2\text{SO}_4$ - $\text{H}_2\text{O}$  Systems at 0.1 MPa and Study: Synthesis, Combustion and formation of benzenesulfonamide and 2-aminobenzothiazole  
2-aminobenzothiazole: Experimental Elevated Temperatures and Pressures: Surface Tensions and Densities of Sulfuric Acid + Dimethylamine + Water  
Combustion energies and formation enthalpies of 2-SH-benzazoles: Liquid-Liquid Equilibria of Nitrobenzene-Inorganic Acid Systems  
Possible precursors and products of deep hydrodesulfurization of gasoline standards and implications for formation of 2-aminobenzothiazoles in the pyrolysis of heavy oil  
Thermodynamic and thermophysical study of 2-aminobenzothiazole and 2-aminobenzothiazole  
Hydantoin and 2-aminobenzothiazole: study of the energetics of hydantoin and 2-aminobenzothiazole  
2-aminobenzothiazole Composition and Density Data for the Sodium Sulfate + Sulfuric Acid + Water System  
Thermodynamic properties of naphthoxazole and naphthothiazole  
Densities and Viscosities of Niacin + 2-Picoline + Sulfuric Acid + Water from 293.15 to 343.15 K  
Rotating-Bomb Combustion Calorimetry and First-Principles Calculations for 1-Ethyl-3-methylimidazolium

## 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

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<https://www.doi.org/10.1021/je1009366>

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

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