L-Cysteine

Other names:	(R)-2-amino-3-mercaptopropanoic acid
	(R)-Cysteine
	2-Amino-3-mercaptopropionic acid
	Cystein
	Cysteine
	Cysteine, L-
	Half-cystine
	L-(+)-Cysteine
	L-Alanine, 3-mercapto-
	L-Cys
	NSC-8746
	Propanoic Acid, 2-amino-3-mercapto-, (R)-
	Thioserine
	«alpha»-Amino-«beta»-thiolpropionic acid
	«beta»-Mercaptoalanine
Inchi:	InChI=1S/C3H7NO2S/c4-2(1-7)3(5)6/h2,7H,1,4H2,(H,5,6)/t2-/m1/s1
InchiKey:	XUJNEKJLAYXESH-UWTATZPHSA-N
Formula:	C3H7NO2S
SMILES:	NC(CS)C(=O)O
Mol. weight [g/mol]:	121.16
CAS:	52-90-4

Physical Properties

Property code	Value	Unit	Source
affp	903.20	kJ/mol	NIST Webbook
basg	869.30	kJ/mol	NIST Webbook
chs	-2229.00 ± 3.00	kJ/mol	NIST Webbook
chs	-2248.90 ± 2.10	kJ/mol	NIST Webbook
chs	-2267.70 ± 2.10	kJ/mol	NIST Webbook
chs	-2248.84 ± 0.55	kJ/mol	NIST Webbook
gf	-197.96	kJ/mol	Joback Method
hf	-303.07	kJ/mol	Joback Method
hfs	-534.08 ± 0.62	kJ/mol	NIST Webbook
hfs	-567.40	kJ/mol	NIST Webbook
hfus	14.93	kJ/mol	Joback Method
hvap	62.69	kJ/mol	Joback Method
log10ws	0.20		Crippen Method

logp	-0.672		Crippen Method
mcvol	86.900	ml/mol	McGowan Method
pc	6696.65	kPa	Joback Method
ss	169.90	J/mol×K	NIST Webbook
tb	549.04	K	Joback Method
tc	760.31	K	Joback Method
tf	339.04	K	Joback Method
vc	0.305	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.08	J/mol×K	549.04	Joback Method
cpg	193.43	J/mol×K	584.25	Joback Method
cpg	199.41	J/mol×K	619.46	Joback Method
cpg	205.04	J/mol×K	654.67	Joback Method
cpg	210.32	J/mol×K	689.89	Joback Method
cpg	215.27	J/mol×K	725.10	Joback Method
cpg	219.90	J/mol×K	760.31	Joback Method
cps	162.30	J/mol×K	297.60	NIST Webbook

Sources

Solvation of Basic and Neutral Amino Acids in Aqueous Electrolytic Solutions: Measurements and Modeling	https://www.doi.org/10.1021/acs.jced.5b00393
Solubility of the Proteinogenic a-Amino Acids in Water, Ethanol, and Ethanol−Water Mixtures:	https://www.doi.org/10.1021/acs.jced.7b00486
Joback Method	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52904&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Synthesis and thermodynamics studies of ionic liquid 1-methyl-3-pentylimidazolium bromide ([C5mim][Br]) with amino acids (L-cysteine and N-acetyl-L-cysteine) at different temperatures:	https://www.doi.org/10.1016/j.jct.2017.03.040

Legend

affp: Proton affinity

basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume