S-Methyl-L-cysteine

Other names: Alanine, 3-(methylthio)-, L-
L-CH3SCH2CH(NH2)COOH
L-Cysteine, S-methyl-
Inchi: InChI=1S/C4H9NO2S/c1-8-2-3(5)4(6)7/h3H,2,5H2,1H3,(H,6,7)/t3-/m1/s1
InchiKey: IDIDJDIHTAOVLG-GSVOUGTGSA-N
Formula: C4H9NO2S
SMILES: CSCC(N)C(=O)O
Mol. weight [g/mol]: 135.19
CAS: 1187-84-4

Physical Properties

Property code	Value	Unit	Source
gf	-185.81	kJ/mol	Joback Method
hf	-320.32	kJ/mol	Joback Method
hfus	17.61	kJ/mol	Joback Method
hvap	64.99	kJ/mol	Joback Method
ie	8.40	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
log10ws	-0.03		Crippen Method
logp	-0.239		Crippen Method
mcvol	100.990	ml/mol	McGowan Method
pc	5367.04	kPa	Joback Method
tb	577.84	K	Joback Method
tc	785.43	K	Joback Method
tf	348.25	K	Joback Method
vc	0.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.62	J/mol×K	577.84	Joback Method
cpg	238.27	J/mol×K	612.44	Joback Method
cpg	245.50	J/mol×K	647.04	Joback Method
cpg	252.32	J/mol×K	681.64	Joback Method

cpg	258.72	J/mol×K	716.24	Joback Method
cpg	264.73	J/mol×K	750.83	Joback Method
cpg	270.33	J/mol×K	785.43	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C1187844&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume