S-propylthiosulfuric acid, 2-amino-2-methyl-

Inchi: InChI=1S/C4H11NO3S2/c1-4(2,5)3-9-10(6,7)8/h3,5H2,1-2H3,(H,6,7,8)
InchiKey: CKFRFNDDOPNLLB-UHFFFAOYSA-N
Formula: C4H11NO3S2
SMILES: CC(C)(N)CSS(=O)(=O)O
Mol. weight [g/mol]: 185.26
CAS: 4039-24-1

Physical Properties

Property code	Value	Unit	Source
gf	-520.15	kJ/mol	Joback Method
hf	-664.56	kJ/mol	Joback Method
hfus	23.50	kJ/mol	Joback Method
hvap	75.97	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	0.260		Crippen Method
mcvol	127.510	ml/mol	McGowan Method
pc	6278.87	kPa	Joback Method
tb	568.96	K	Joback Method
tc	769.30	K	Joback Method
tf	354.30	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.91	J/mol×K	568.96	Joback Method
cpg	308.33	J/mol×K	602.35	Joback Method
cpg	317.17	J/mol×K	635.74	Joback Method
cpg	325.42	J/mol×K	669.13	Joback Method
cpg	333.10	J/mol×K	702.52	Joback Method
cpg	340.21	J/mol×K	735.91	Joback Method
cpg	346.77	J/mol×K	769.30	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C4039241&Units=SI

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
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