1-(Methylthio)-1-propanethiol

Inchi: InChI=1S/C4H10S2/c1-3-4(5)6-2/h4-5H,3H2,1-2H3
InchiKey: CRBTVRXQYRRGOE-UHFFFAOYSA-N
Formula: C4H10S2
SMILES: CCC(S)SC
Mol. weight [g/mol]: 122.25

Physical Properties

Property code	Value	Unit	Source
gf	42.87	kJ/mol	Joback Method
hf	-50.82	kJ/mol	Joback Method
hfus	10.76	kJ/mol	Joback Method
hvap	37.66	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.015		Crippen Method
mcvol	99.920	ml/mol	McGowan Method
pc	4368.40	kPa	Joback Method
rinpol	913.90		NIST Webbook
tb	422.12	K	Joback Method
tc	645.85	K	Joback Method
tf	190.70	K	Joback Method
vc	0.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.85	J/mol×K	422.12	Joback Method
cpg	184.60	J/mol×K	459.41	Joback Method
cpg	193.91	J/mol×K	496.70	Joback Method
cpg	202.78	J/mol×K	533.98	Joback Method
cpg	211.21	J/mol×K	571.27	Joback Method
cpg	219.21	J/mol×K	608.56	Joback Method
cpg	226.78	J/mol×K	645.85	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=R494530&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume