1,3-Bis-(methylthio)-2-methoxypropane

Other names: Propane, 2-methoxy-1,3-bis(methylthio)-
2-methoxy-1,3-bis(methylthio)propane
Inchi: InChI=1S/C6H14OS2/c1-7-6(4-8-2)5-9-3/h6H,4-5H2,1-3H3
InchiKey: MOISORXUYSHXRU-UHFFFAOYSA-N
Formula: C6H14OS2
SMILES: COC(CSC)CSC
Mol. weight [g/mol]: 166.31
CAS: 31805-84-2

Physical Properties

Property code	Value	Unit	Source
gf	-41.56	kJ/mol	Joback Method
hf	-220.93	kJ/mol	Joback Method
hfus	17.22	kJ/mol	Joback Method
hvap	44.61	kJ/mol	Joback Method
log10ws	-1.30		Crippen Method
logp	1.727		Crippen Method
mcvol	133.970	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
tb	496.22	K	Joback Method
tc	711.42	K	Joback Method
tf	233.41	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.90	J/mol×K	496.22	Joback Method
cpg	289.37	J/mol×K	532.09	Joback Method
cpg	301.34	J/mol×K	567.95	Joback Method
cpg	312.80	J/mol×K	603.82	Joback Method
cpg	323.73	J/mol×K	639.69	Joback Method
cpg	334.12	J/mol×K	675.55	Joback Method
cpg	343.95	J/mol×K	711.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31805842&Units=SI
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

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