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

Other names: 2-Propanol, 1,3-bis(methylthio)-
1,3-bis(methylthio)propan-2-ol
Inchi: InChI=1S/C5H12OS2/c1-7-3-5(6)4-8-2/h5-6H,3-4H2,1-2H3
InchiKey: BTQNSLFPJKRBQK-UHFFFAOYSA-N
Formula: C5H12OS2
SMILES: CSCC(O)CSC
Mol. weight [g/mol]: 152.28
CAS: 31805-83-1

Physical Properties

Property code	Value	Unit	Source
gf	-81.80	kJ/mol	Joback Method
hf	-220.30	kJ/mol	Joback Method
hfus	17.53	kJ/mol	Joback Method
hvap	56.65	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	1.073		Crippen Method
mcvol	119.880	ml/mol	McGowan Method
pc	4088.15	kPa	Joback Method
tb	543.10	K	Joback Method
tc	748.61	K	Joback Method
tf	260.73	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.77	J/mol×K	543.10	Joback Method
cpg	267.50	J/mol×K	577.35	Joback Method
cpg	276.77	J/mol×K	611.60	Joback Method
cpg	285.57	J/mol×K	645.85	Joback Method
cpg	293.92	J/mol×K	680.10	Joback Method
cpg	301.80	J/mol×K	714.36	Joback Method
cpg	309.22	J/mol×K	748.61	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	374.50 ± 0.50	K	0.50	NIST Webbook

Sources

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=C31805831&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume