1,3-Propanediol, 2-(hydroxymethyl)-2-methyl-, tris(mercaptoacetae)

Other names: 2-[[(mercaptoacetyl)oxy]methyl]-2-methyl-1,3-propanediyl bis(mercaptoacetate)
Inchi: InChI=1S/C11H18O6S3/c1-11(5-15-8(12)2-18,6-16-9(13)3-19)7-17-10(14)4-20/h18-20H,
InchiKey: OMGUQSBVDSVSQB-UHFFFAOYSA-N
Formula: C11H18O6S3
SMILES: CC(COC(=O)CS)(COC(=O)CS)COC(=O)CS
Mol. weight [g/mol]: 342.45
CAS: 10193-98-3

Physical Properties

Property code	Value	Unit	Source
gf	-569.01	kJ/mol	Joback Method
hf	-898.08	kJ/mol	Joback Method
hfus	37.32	kJ/mol	Joback Method
hvap	86.46	kJ/mol	Joback Method
log10ws	-0.99		Crippen Method
logp	0.412		Crippen Method
mcvol	237.220	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
tb	865.30	K	Joback Method
tc	1100.44	K	Joback Method
tf	542.01	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.28	J/mol×K	865.30	Joback Method
cpg	665.91	J/mol×K	904.49	Joback Method
cpg	675.38	J/mol×K	943.68	Joback Method
cpg	683.69	J/mol×K	982.87	Joback Method
cpg	690.86	J/mol×K	1022.06	Joback Method
cpg	696.87	J/mol×K	1061.25	Joback Method
cpg	701.75	J/mol×K	1100.44	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=C10193983&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