Pentaerythritol, tetrakis(mercaptoacetate)

Other names: 2,2-bis[[(mercaptoacetyl)oxy]methyl]-1,3-propanediyl bis(mercaptoacetate)
Inchi: InChI=1S/C13H20O8S4/c14-9(1-22)18-5-13(6-19-10(15)2-23,7-20-11(16)3-24)8-21-12(1
InchiKey: RUDUCNPHDIMQCY-UHFFFAOYSA-N
Formula: C13H20O8S4
SMILES: O=C(CS)OCC(COC(=O)CS)(COC(=O)CS)COC(=O)CS
Mol. weight [g/mol]: 432.55
CAS: 10193-99-4

Physical Properties

Property code	Value	Unit	Source
gf	-756.70	kJ/mol	Joback Method
hf	-1145.68	kJ/mol	Joback Method
hfus	49.33	kJ/mol	Joback Method
hvap	106.81	kJ/mol	Joback Method
log10ws	-0.76		Crippen Method
logp	-0.135		Crippen Method
mcvol	289.190	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
tb	1050.21	K	Joback Method
tc	1299.51	K	Joback Method
tf	673.17	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	832.09	J/mol×K	1050.21	Joback Method
cpg	837.74	J/mol×K	1091.76	Joback Method
cpg	841.73	J/mol×K	1133.31	Joback Method
cpg	844.04	J/mol×K	1174.86	Joback Method
cpg	844.66	J/mol×K	1216.41	Joback Method
cpg	843.59	J/mol×K	1257.96	Joback Method
cpg	840.82	J/mol×K	1299.51	Joback Method

Sources

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=C10193994&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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