1,3-Bis(2-hydroxyethylthio)propane

Inchi: InChI=1S/C7H16O2S2/c8-2-6-10-4-1-5-11-7-3-9/h8-9H,1-7H2
InchiKey: JIJWGPUMOGBVMQ-UHFFFAOYSA-N
Formula: C7H16O2S2
SMILES: OCCSCCCSCCO
Mol. weight [g/mol]: 196.33
CAS: 16260-48-3

Physical Properties

Property code	Value	Unit	Source
gf	-199.34	kJ/mol	Joback Method
hf	-408.53	kJ/mol	Joback Method
hfus	30.32	kJ/mol	Joback Method
hvap	78.17	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	0.828		Crippen Method
mcvol	153.930	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
rinpol	1809.00		NIST Webbook
tb	681.48	K	Joback Method
tc	868.07	K	Joback Method
tf	359.09	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.63	J/mol×K	681.48	Joback Method
cpg	405.23	J/mol×K	712.58	Joback Method
cpg	414.32	J/mol×K	743.68	Joback Method
cpg	422.91	J/mol×K	774.78	Joback Method
cpg	431.02	J/mol×K	805.87	Joback Method
cpg	438.64	J/mol×K	836.97	Joback Method
cpg	445.79	J/mol×K	868.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16260483&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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