Ethanol, 2,2'-[methylenebis(thio)]bis-

Other names: Bis(2-hydroxyethylthio)methane
2,2'-(Methylenebis(thio))bisethanol
3,5-Dithiaheptane-1,7-diol
Inchi: InChI=1S/C5H12O2S2/c6-1-3-8-5-9-4-2-7/h6-7H,1-5H2
InchiKey: GAECBAMNQFGJIM-UHFFFAOYSA-N
Formula: C5H12O2S2
SMILES: OCCSCSCCO
Mol. weight [g/mol]: 168.28
CAS: 44860-68-6

Physical Properties

Property code	Value	Unit	Source
gf	-216.18	kJ/mol	Joback Method
hf	-367.25	kJ/mol	Joback Method
hfus	25.14	kJ/mol	Joback Method
hvap	73.72	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	0.395		Crippen Method
mcvol	125.750	ml/mol	McGowan Method
pc	4565.38	kPa	Joback Method
rinpol	1574.00		NIST Webbook
rinpol	1574.00		NIST Webbook
tb	635.72	K	Joback Method
tc	825.45	K	Joback Method
tf	336.55	K	Joback Method
vc	0.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.48	J/mol×K	635.72	Joback Method
cpg	307.51	J/mol×K	667.34	Joback Method
cpg	315.13	J/mol×K	698.96	Joback Method
cpg	322.35	J/mol×K	730.58	Joback Method

cpg	329.16	J/mol×K	762.21	Joback Method
cpg	335.58	J/mol×K	793.83	Joback Method
cpg	341.60	J/mol×K	825.45	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=C44860686&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume