1-(2-Hydroxyethylthio)-4-(2-hydroxyethyldithio)bu

Inchi: InChI=1S/C8H18O2S3/c9-3-7-11-5-1-2-6-12-13-8-4-10/h9-10H,1-8H2
InchiKey: BNWPXFUBFMWJGZ-UHFFFAOYSA-N
Formula: C8H18O2S3
SMILES: OCCSCCCCSSCCO
Mol. weight [g/mol]: 242.42

Physical Properties

Property code	Value	Unit	Source
gf	-157.80	kJ/mol	Joback Method
hf	-387.30	kJ/mol	Joback Method
hfus	37.04	kJ/mol	Joback Method
hvap	87.21	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	1.866		Crippen Method
mcvol	184.370	ml/mol	McGowan Method
pc	3261.58	kPa	Joback Method
rinpol	1929.00		NIST Webbook
tb	773.14	K	Joback Method
tc	972.41	K	Joback Method
tf	404.76	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.53	J/mol×K	773.14	Joback Method
cpg	504.44	J/mol×K	806.35	Joback Method
cpg	513.69	J/mol×K	839.56	Joback Method
cpg	522.28	J/mol×K	872.77	Joback Method
cpg	530.22	J/mol×K	905.98	Joback Method
cpg	537.50	J/mol×K	939.19	Joback Method
cpg	544.14	J/mol×K	972.41	Joback Method

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=R500997&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume