N,n'-ethylenebis(3-mercaptopropionamide)

Inchi: InChI=1S/C8H16N2O2S2/c11-7(1-5-13)9-3-4-10-8(12)2-6-14/h13-14H,1-6H2,(H,9,11)(H,
InchiKey: BSICYDQQORWGMR-UHFFFAOYSA-N
Formula: C8H16N2O2S2
SMILES: O=C(CCS)NCCNC(=O)CCS
Mol. weight [g/mol]: 236.35
CAS: 818-41-7

Physical Properties

Property code	Value	Unit	Source
gf	-3.80	kJ/mol	Joback Method
hf	-249.71	kJ/mol	Joback Method
hfus	37.96	kJ/mol	Joback Method
hvap	73.24	kJ/mol	Joback Method
log10ws	-1.24		Crippen Method
logp	-0.141		Crippen Method
mcvol	179.380	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
tb	716.24	K	Joback Method
tc	936.42	K	Joback Method
tf	458.02	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.26	J/mol×K	716.24	Joback Method
cpg	475.84	J/mol×K	752.94	Joback Method
cpg	486.63	J/mol×K	789.63	Joback Method
cpg	496.65	J/mol×K	826.33	Joback Method
cpg	505.94	J/mol×K	863.03	Joback Method
cpg	514.52	J/mol×K	899.73	Joback Method
cpg	522.43	J/mol×K	936.42	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=C818417&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume