N,n'-ethylenebis(2-mercaptopropionamide)

Inchi: InChI=1S/C8H16N2O2S2/c1-5(13)7(11)9-3-4-10-8(12)6(2)14/h5-6,13-14H,3-4H2,1-2H3,(
InchiKey: NQBOCGBWMCQBAA-UHFFFAOYSA-N
Formula: C8H16N2O2S2
SMILES: CC(S)C(=O)NCCNC(=O)C(C)S
Mol. weight [g/mol]: 236.35
CAS: 687-72-9

Physical Properties

Property code	Value	Unit	Source
gf	-8.68	kJ/mol	Joback Method
hf	-260.27	kJ/mol	Joback Method
hfus	30.91	kJ/mol	Joback Method
hvap	72.46	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	-0.145		Crippen Method
mcvol	179.380	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
tb	715.36	K	Joback Method
tc	943.75	K	Joback Method
tf	428.02	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.43	J/mol×K	715.36	Joback Method
cpg	477.48	J/mol×K	753.42	Joback Method
cpg	488.65	J/mol×K	791.49	Joback Method
cpg	498.98	J/mol×K	829.55	Joback Method
cpg	508.49	J/mol×K	867.62	Joback Method
cpg	517.22	J/mol×K	905.68	Joback Method
cpg	525.20	J/mol×K	943.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C687729&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume