N,n'-ethylenebis(mercaptoacetamide)

Inchi: InChI=1S/C6H12N2O2S2/c9-5(3-11)7-1-2-8-6(10)4-12/h11-12H,1-4H2,(H,7,9)(H,8,10)
InchiKey: SQPIKOWZWIINCK-UHFFFAOYSA-N
Formula: C6H12N2O2S2
SMILES: O=C(CS)NCCNC(=O)CS
Mol. weight [g/mol]: 208.30
CAS: 692-93-3

Physical Properties

Property code	Value	Unit	Source
gf	-20.64	kJ/mol	Joback Method
hf	-208.43	kJ/mol	Joback Method
hfus	32.78	kJ/mol	Joback Method
hvap	68.79	kJ/mol	Joback Method
log10ws	-0.41		Crippen Method
logp	-0.922		Crippen Method
mcvol	151.200	ml/mol	McGowan Method
pc	4362.63	kPa	Joback Method
tb	670.48	K	Joback Method
tc	898.51	K	Joback Method
tf	435.48	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.82	J/mol×K	670.48	Joback Method
cpg	375.06	J/mol×K	708.49	Joback Method
cpg	384.57	J/mol×K	746.49	Joback Method
cpg	393.39	J/mol×K	784.50	Joback Method
cpg	401.54	J/mol×K	822.50	Joback Method
cpg	409.04	J/mol×K	860.51	Joback Method
cpg	415.92	J/mol×K	898.51	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=C692933&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