N-(2-aminoethyl) mercaptoacetamide

Inchi: InChI=1S/C4H10N2OS/c5-1-2-6-4(7)3-8/h8H,1-3,5H2,(H,6,7)
InchiKey: TZUUVDLWMJGBND-UHFFFAOYSA-N
Formula: C4H10N2OS
SMILES: NCCNC(=O)CS
Mol. weight [g/mol]: 134.20
CAS: 62-47-5

Physical Properties

Property code	Value	Unit	Source
gf	39.11	kJ/mol	Joback Method
hf	-112.73	kJ/mol	Joback Method
hfus	22.05	kJ/mol	Joback Method
hvap	55.06	kJ/mol	Joback Method
log10ws	0.03		Crippen Method
logp	-1.009		Crippen Method
mcvol	105.100	ml/mol	McGowan Method
pc	5065.79	kPa	Joback Method
tb	530.35	K	Joback Method
tc	749.81	K	Joback Method
tf	357.15	K	Joback Method
vc	0.384	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.90	J/mol×K	530.35	Joback Method
cpg	239.14	J/mol×K	566.93	Joback Method
cpg	247.86	J/mol×K	603.50	Joback Method
cpg	256.07	J/mol×K	640.08	Joback Method
cpg	263.78	J/mol×K	676.66	Joback Method
cpg	271.01	J/mol×K	713.23	Joback Method
cpg	277.78	J/mol×K	749.81	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62475&Units=SI

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