N-(3-aminopropyl)-2-mercaptopropionamide

Inchi: InChI=1S/C6H14N2OS/c1-5(10)6(9)8-4-2-3-7/h5,10H,2-4,7H2,1H3,(H,8,9)
InchiKey: SZRLWIWKHLYZHF-UHFFFAOYSA-N
Formula: C6H14N2OS
SMILES: CC(S)C(=O)NCCCN
Mol. weight [g/mol]: 162.25
CAS: 816-77-3

Physical Properties

Property code	Value	Unit	Source
gf	53.51	kJ/mol	Joback Method
hf	-159.29	kJ/mol	Joback Method
hfus	23.71	kJ/mol	Joback Method
hvap	59.12	kJ/mol	Joback Method
log10ws	-0.92		Crippen Method
logp	-0.230		Crippen Method
mcvol	133.280	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
tb	575.67	K	Joback Method
tc	792.32	K	Joback Method
tf	364.69	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.89	J/mol×K	575.67	Joback Method
cpg	329.54	J/mol×K	611.78	Joback Method
cpg	340.51	J/mol×K	647.89	Joback Method
cpg	350.83	J/mol×K	683.99	Joback Method
cpg	360.52	J/mol×K	720.10	Joback Method
cpg	369.60	J/mol×K	756.21	Joback Method
cpg	378.10	J/mol×K	792.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C816773&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

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