Belta-mercaptopropionamide

Inchi: InChI=1S/C3H7NOS/c4-3(5)1-2-6/h6H,1-2H2,(H2,4,5)
InchiKey: JLSJEUQOXVVCPN-UHFFFAOYSA-N
Formula: C3H7NOS
SMILES: N=C(O)CCS
Mol. weight [g/mol]: 105.16
CAS: 763-35-9

Physical Properties

Property code	Value	Unit	Source
gf	70.55	kJ/mol	Joback Method
hf	-20.67	kJ/mol	Joback Method
hvap	57.77	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	0.842		Crippen Method
mcvol	81.030	ml/mol	McGowan Method
tb	507.42	K	Joback Method
tf	289.63	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.56	J/mol×K	507.42	Joback Method
cpg	41.72	J/mol×K	100.12	Joback Method
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Sources

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=C763359&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point