Urea, (2-mercaptoethyl)-

Inchi: InChI=1S/C3H8N2OS/c4-3(6)5-1-2-7/h7H,1-2H2,(H3,4,5,6)
InchiKey: XLCDSNFXNIFAJK-UHFFFAOYSA-N
Formula: C3H8N2OS
SMILES: NC(=O)NCCS
Mol. weight [g/mol]: 120.17

Physical Properties

Property code	Value	Unit	Source
gf	30.69	kJ/mol	Joback Method
hf	-92.09	kJ/mol	Joback Method
hfus	19.46	kJ/mol	Joback Method
hvap	52.83	kJ/mol	Joback Method
log10ws	-0.53		Crippen Method
logp	-0.415		Crippen Method
mcvol	91.010	ml/mol	McGowan Method
pc	5836.07	kPa	Joback Method
tb	507.47	K	Joback Method
tc	730.75	K	Joback Method
tf	345.88	K	Joback Method
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.99	J/mol×K	507.47	Joback Method
cpg	196.96	J/mol×K	544.68	Joback Method
cpg	204.48	J/mol×K	581.90	Joback Method
cpg	211.54	J/mol×K	619.11	Joback Method
cpg	218.18	J/mol×K	656.33	Joback Method
cpg	224.39	J/mol×K	693.54	Joback Method
cpg	230.20	J/mol×K	730.75	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=B6007394&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