Thiourea, N,N-dimethyl-

Other names:	Urea, 1,1-dimethyl-2-thio- N,N-Dimethylthiourea 1,1-Dimethylthiourea 1,1-dimethyl-2-thiourea
Inchi:	InChI=1S/C3H8N2S/c1-5(2)3(4)6/h1-2H3,(H2,4,6)
InchiKey:	ZQGWBPQBZHMUFG-UHFFFAOYSA-N
Formula:	C3H8N2S
SMILES:	CN(C)C(N)=S
Mol. weight [g/mol]:	104.17
CAS:	6972-05-0

Physical Properties

Property code	Value	Unit	Source
gf	268.67	kJ/mol	Joback Method
hf	142.57	kJ/mol	Joback Method
hfus	16.35	kJ/mol	Joback Method
hvap	41.69	kJ/mol	Joback Method
ie	8.34 ± 0.05	eV	NIST Webbook
log10ws	-0.43		Crippen Method
logp	-0.208		Crippen Method
mcvol	85.140	ml/mol	McGowan Method
pc	5414.53	kPa	Joback Method
tb	423.05	K	Joback Method
tc	636.07	K	Joback Method
tf	273.57	K	Joback Method
vc	0.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	157.48	J/mol×K	423.05	Joback Method
cpg	165.99	J/mol×K	458.55	Joback Method
cpg	173.86	J/mol×K	494.06	Joback Method
cpg	181.11	J/mol×K	529.56	Joback Method

cpg	187.80	J/mol×K	565.07	Joback Method
cpg	193.99	J/mol×K	600.57	Joback Method
cpg	199.71	J/mol×K	636.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6972050&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
ie:	Ionization energy
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