Thiourea, N,N'-dimethyl-

Other names:	(CH3NH)2CS
	1,3-Dimethyl-2-thiourea
	1,3-dimethylthiourea
	Dimethylthiocarbamide
	N,N'-dimethylthiourea
	Urea, 1,3-dimethyl-2-thio-
	sym-Dimethylthiourea
	thiourea, 1,3-dimethyl-
Inchi:	InChI=1S/C3H8N2S/c1-4-3(6)5-2/h1-2H3,(H2,4,5,6)
InchiKey:	VLCDUOXHFNUCKK-UHFFFAOYSA-N
Formula:	C3H8N2S
SMILES:	CNC(=S)NC
Mol. weight [g/mol]:	104.17
CAS:	534-13-4

Physical Properties

Property code	Value	Unit	Source
affp	926.00	kJ/mol	NIST Webbook
basg	895.10	kJ/mol	NIST Webbook
gf	270.22	kJ/mol	Joback Method
hf	148.19	kJ/mol	Joback Method
hfus	18.33	kJ/mol	Joback Method
hsub	107.30 ± 4.00	kJ/mol	NIST Webbook
hsub	112.00 ± 3.00	kJ/mol	NIST Webbook
hvap	41.87	kJ/mol	Joback Method
ie	8.17 ± 0.05	eV	NIST Webbook
ie	8.08 ± 0.03	eV	NIST Webbook
log10ws	-0.80		Crippen Method
logp	-0.290		Crippen Method
mcvol	85.140	ml/mol	McGowan Method
pc	5190.64	kPa	Joback Method
tb	438.42	K	Joback Method
tc	646.02	K	Joback Method
tf	337.00 ± 0.10	K	NIST Webbook
vc	0.309	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.72	J/mol×K	576.82	Joback Method
cpg	192.86	J/mol×K	611.42	Joback Method
cpg	157.38	J/mol×K	438.42	Joback Method
cpg	165.51	J/mol×K	473.02	Joback Method
cpg	173.09	J/mol×K	507.62	Joback Method
cpg	180.15	J/mol×K	542.22	Joback Method
cpg	198.59	J/mol×K	646.02	Joback Method
hfust	13.71	kJ/mol	337.00	NIST Webbook
hfust	12.70	kJ/mol	336.90	NIST Webbook
hsubt	108.00 ± 3.00	kJ/mol	361.00	NIST Webbook
hvapt	93.00 ± 4.00	kJ/mol	358.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C534134&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Apparent Molar Volumes and Expansibilities of Thiourea, 1,3-Dimethylurea, and 1,3-Dimethylthiourea in Water at Temperatures from T = (278.15 to 318.15) K and Atmospheric Pressure:	https://www.doi.org/10.1021/je301203z
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions

hvapt:	Enthalpy of vaporization at a given temperature
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