Thiourea, methyl-

Other names:	Methylthiocarbamide
	Urea, 1-methyl-2-thio-
	Methylthiourea
	N-Methylthiocarbamide
	N-Methylthiourea
	1-Methyl-2-thiourea
	1-Methylthiocarbamide
	1-Methylthiourea
	Monomethylthiourea
	NSC 30213
	Pseudourea, 1-methyl-2-thio-
	methyl-2-thiourea
Inchi:	InChI=1S/C2H6N2S/c1-4-2(3)5/h1H3,(H3,3,4,5)
InchiKey:	KQJQICVXLJTWQD-UHFFFAOYSA-N
Formula:	C2H6N2S
SMILES:	CNC(N)=S
Mol. weight [g/mol]:	90.15
CAS:	598-52-7

Physical Properties

Property code	Value	Unit	Source
gf	238.86	kJ/mol	Joback Method
hf	149.15	kJ/mol	Joback Method
hfus	15.83	kJ/mol	Joback Method
hsub	113.00 ± 3.00	kJ/mol	NIST Webbook
hvap	43.85	kJ/mol	Joback Method
ie	8.29 ± 0.05	eV	NIST Webbook
log10ws	-0.63		Crippen Method
logp	-0.551		Crippen Method
mcvol	71.050	ml/mol	McGowan Method
pc	6420.53	kPa	Joback Method
tb	437.90	K	Joback Method
tc	659.56	K	Joback Method
tf	282.49	K	Joback Method
vc	0.247	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	128.46	J/mol×K	437.90	Joback Method
cpg	134.84	J/mol×K	474.84	Joback Method
cpg	140.71	J/mol×K	511.79	Joback Method
cpg	146.10	J/mol×K	548.73	Joback Method
cpg	151.07	J/mol×K	585.67	Joback Method
cpg	155.65	J/mol×K	622.62	Joback Method
cpg	159.89	J/mol×K	659.56	Joback Method
hfust	19.46	kJ/mol	392.40	NIST Webbook
hsubt	111.00 ± 3.00	kJ/mol	381.00	NIST Webbook

Sources

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=C598527&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
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
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