Thiourea, trimethyl-

Other names:	Urea, 1,1,3-trimethyl-2-thio-
	N,N,N'-Trimethylthiourea
	Thiate E
	Trimethylthiourea
	1,1,3-Trimethylthiourea
	1,3,3-Trimethylthiourea
	NCI-C02186
	1,1,3-Trimethyl-2-thiourea
	NSC 153385
	Thiourea, N,N,N'-trimethyl-
	trimethyl-2-thiourea
Inchi:	InChI=1S/C4H10N2S/c1-5-4(7)6(2)3/h1-3H3,(H,5,7)
InchiKey:	JAEZSIYNWDWMMN-UHFFFAOYSA-N
Formula:	C4H10N2S
SMILES:	CNC(=S)N(C)C
Mol. weight [g/mol]:	118.20
CAS:	2489-77-2

Physical Properties

Property code	Value	Unit	Source
gf	300.03	kJ/mol	Joback Method
hf	141.61	kJ/mol	Joback Method
hfus	18.84	kJ/mol	Joback Method
hvap	39.71	kJ/mol	Joback Method
ie	7.93 ± 0.05	eV	NIST Webbook
log10ws	-0.60		Crippen Method
logp	0.052		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
pc	4450.38	kPa	Joback Method
tb	423.57	K	Joback Method
tc	623.12	K	Joback Method
tf	254.24	K	Joback Method
vc	0.348	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.48	J/mol×K	423.57	Joback Method
cpg	195.58	J/mol×K	456.83	Joback Method
cpg	205.00	J/mol×K	490.09	Joback Method
cpg	213.79	J/mol×K	523.34	Joback Method
cpg	221.99	J/mol×K	556.60	Joback Method
cpg	229.65	J/mol×K	589.86	Joback Method
cpg	236.80	J/mol×K	623.12	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2489772&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