

Thiourea, N,N'-diethyl-

Other names:	1,3-Diethyl-2-Thiourea
	1,3-Diethylthiourea
	Diethyl-2-thiourea
	N,N'-Diethylthiocarbamide
	N,N'-Diethylthiourea
	N,N'-Diethylthiourea (sym)
	NCI-C03816
	NSC 3507
	Pennzone E
	Thiate H
	U 15030
	USAF EK-1803
	Urea, 1,3-diethyl-2-thio-
Inchi:	InChI=1S/C5H12N2S/c1-3-6-5(8)7-4-2/h3-4H2,1-2H3,(H2,6,7,8)
InchiKey:	FLVIGYVXZHLUHP-UHFFFAOYSA-N
Formula:	C5H12N2S
SMILES:	CCNC(=S)NCC
Mol. weight [g/mol]:	132.23
CAS:	105-55-5

Physical Properties

Property code	Value	Unit	Source
gf	287.06	kJ/mol	Joback Method
hf	106.91	kJ/mol	Joback Method
hfus	23.51	kJ/mol	Joback Method
hsub	120.20 ± 3.00	kJ/mol	NIST Webbook
hsub	122.00 ± 3.00	kJ/mol	NIST Webbook
hvap	46.33	kJ/mol	Joback Method
ie	7.98 ± 0.05	eV	NIST Webbook
log10ws	-1.46		Estimated Solubility Method
log10ws	-1.46		Aqueous Solubility Prediction Method
logp	0.490		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
pc	4005.77	kPa	Joback Method
tb	484.18	K	Joback Method

tc	686.47	K	Joback Method
tf	350.60 ± 0.10	K	NIST Webbook
tf	350.65	K	Aqueous Solubility Prediction Method
vc	0.421	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.13	J/mol×K	652.76	Joback Method
cpg	235.39	J/mol×K	484.18	Joback Method
cpg	245.94	J/mol×K	517.90	Joback Method
cpg	255.85	J/mol×K	551.61	Joback Method
cpg	265.16	J/mol×K	585.33	Joback Method
cpg	273.91	J/mol×K	619.04	Joback Method
cpg	289.86	J/mol×K	686.47	Joback Method
hfust	17.14	kJ/mol	350.50	NIST Webbook
hvapt	101.00 ± 3.00	kJ/mol	367.50	NIST Webbook
rhos	1120.00	kg/m ³	293.00	Solid-Liquid Phase Equilibrium and Thermodynamic Analysis of N,N'-Diethylthiourea in Different Solvent Systems

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105555&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solid-Liquid Phase Equilibrium and Thermodynamic Analysis of N,N'-Diethylthiourea in Different Solvent Systems:	https://www.doi.org/10.1021/acs.jced.9b00854
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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
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
rhos:	Solid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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