

Thiourea, N,N'-bis(1-methylethyl)-

Other names:	Urea, 1,3-diisopropyl-2-thio-Diisopropylthiourea N,N'-Diisopropylthiourea 1,3-Diisopropyl-2-thiourea 1,3-Diisopropylthiourea sym-Diisopropylthiourea
Inchi:	InChI=1S/C7H16N2S/c1-5(2)8-7(10)9-6(3)4/h5-6H,1-4H3,(H2,8,9,10)
InchiKey:	KREOCUNMMFZOOS-UHFFFAOYSA-N
Formula:	C7H16N2S
SMILES:	CC(C)NC(=S)NC(C)C
Mol. weight [g/mol]:	160.28
CAS:	2986-17-6

Physical Properties

Property code	Value	Unit	Source
gf	299.02	kJ/mol	Joback Method
hf	55.07	kJ/mol	Joback Method
hfus	21.64	kJ/mol	Joback Method
hvap	50.00	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	1.267		Crippen Method
mcvol	141.500	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
tb	529.06	K	Joback Method
tc	734.53	K	Joback Method
tf	278.24	K	Joback Method
vc	0.521	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.03	J/mol×K	529.06	Joback Method
cpg	335.19	J/mol×K	563.30	Joback Method
cpg	347.55	J/mol×K	597.55	Joback Method

cpg	359.18	J/mol×K	631.79	Joback Method
cpg	370.11	J/mol×K	666.04	Joback Method
cpg	380.40	J/mol×K	700.28	Joback Method
cpg	390.09	J/mol×K	734.53	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C2986176&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
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

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