1,3-di-o-Tolyl-2-thiourea

Other names:	N,N'-di-o-Tolylthiourea Thiourea, N,N'-bis(2-methylphenyl)- sym-Di-o-tolylthiourea Carbanilide, 2,2'-dimethylthio- Di-o-toluylthiourea Di-o-tolylthiourea N,N'-Bis(2-methylphenyl)thiourea Urea, 1,3-bis(o-tolyl)-2-thio- USAF EK-1651 1,3-Bis(o-tolyl)thiourea 1,3-Di-o-tolylthiourea 2,2'-Dimethylthiocarbanilide 1,3-Di-o-tolylthiomocovina 1,3-Bis(o-tolyl)-2-thiourea Thiourea, 1,3-di-O-tolyl- Carbanilide, O,O'-dimethylthio- NSC 119321
Inchi:	InChI=1S/C15H16N2S/c1-11-7-3-5-9-13(11)16-15(18)17-14-10-6-4-8-12(14)2/h3-10H,1-2
InchiKey:	KWPNNZKRAQDVPZ-UHFFFAOYSA-N
Formula:	C15H16N2S
SMILES:	Cc1ccccc1NC(=S)Nc1ccccc1C
Mol. weight [g/mol]:	256.37
CAS:	137-97-3

Physical Properties

Property code	Value	Unit	Source
gf	576.82	kJ/mol	Joback Method
hf	350.63	kJ/mol	Joback Method
hfus	36.71	kJ/mol	Joback Method
hvap	74.46	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.112		Crippen Method
mcvol	206.700	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
tb	776.30	K	Joback Method
tc	1028.41	K	Joback Method
tf	476.28	K	Joback Method

vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	554.32	J/mol×K	776.30	Joback Method
cpg	568.41	J/mol×K	818.32	Joback Method
cpg	581.44	J/mol×K	860.34	Joback Method
cpg	593.53	J/mol×K	902.35	Joback Method
cpg	604.81	J/mol×K	944.37	Joback Method
cpg	615.43	J/mol×K	986.39	Joback Method
cpg	625.50	J/mol×K	1028.41	Joback Method

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=C137973&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
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