

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-tolylthiourea
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-

InchiKey:

KWPNNZKRAQDVPZ-UHFFFAOYSA-N

Formula:

C15H16N2S

SMILES:

Cc1cccc1NC(=S)Nc1cccc1C

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

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=C137973&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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