

Thiourea, N,N'-bis(2-ethylphenyl)-

Other names:	2,2'-Diethylthiocarbanilide 1,3-(Bis(2-ethylphenyl))thiourea
Inchi:	InChI=1S/C17H20N2S/c1-3-13-9-5-7-11-15(13)18-17(20)19-16-12-8-6-10-14(16)4-2/h5-1
InchiKey:	WYMLGVPROUZGCI-UHFFFAOYSA-N
Formula:	C17H20N2S
SMILES:	CCc1ccccc1NC(=S)Nc1ccccc1CC
Mol. weight [g/mol]:	284.42
CAS:	5395-94-8

Physical Properties

Property code	Value	Unit	Source
gf	593.66	kJ/mol	Joback Method
hf	309.35	kJ/mol	Joback Method
hfus	41.89	kJ/mol	Joback Method
hvap	78.91	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.620		Crippen Method
mvol	234.880	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
tb	822.06	K	Joback Method
tc	1064.51	K	Joback Method
tf	498.82	K	Joback Method
vc	0.877	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.69	J/molxK	822.06	Joback Method
cpg	678.46	J/molxK	862.47	Joback Method
cpg	692.23	J/molxK	902.88	Joback Method
cpg	705.10	J/molxK	943.28	Joback Method
cpg	717.22	J/molxK	983.69	Joback Method
cpg	728.70	J/molxK	1024.10	Joback Method
cpg	739.68	J/molxK	1064.51	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=C5395948&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

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