

2,2'-Diethylthiocarbanilide

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]:	284.43

Physical Properties

Property code	Value	Unit	Source
af	0.7208		Cheméo Relay (1.0)
gf	593.66	kJ/mol	Joback Method
hf	141.68	kJ/mol	Cheméo Relay (1.0)
hfus	41.89	kJ/mol	Joback Method
hvap	114.46	kJ/mol	Cheméo Relay (1.0)
ie	7.30	eV	Cheméo Relay (1.0)
log10ws	-5.56		Cheméo Relay (1.0)
logp	4.620		Crippen Method
mcvol	234.880	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
tb	630.04	K	Cheméo Relay (1.0)
tc	972.54	K	Cheméo Relay (1.0)
tf	430.76	K	Cheméo Relay (1.0)
vc	0.812	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.69	J/mol×K	822.06	Joback Method
cpg	678.46	J/mol×K	862.47	Joback Method
cpg	692.23	J/mol×K	902.88	Joback Method
cpg	705.10	J/mol×K	943.28	Joback Method
cpg	717.22	J/mol×K	983.69	Joback Method
cpg	728.70	J/mol×K	1024.10	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5395948&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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