

Urea, N,N-diphenyl-N'-(3-methylbutyl)-

Inchi:	InChI=1S/C18H22N2O/c1-15(2)13-14-19-18(21)20(16-9-5-3-6-10-16)17-11-7-4-8-12-17/
InchiKey:	AVFIAQSZHXFAMB-UHFFFAOYSA-N
Formula:	C18H22N2O
SMILES:	CC(C)CCN=C(O)N(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	282.38

Physical Properties

Property code	Value	Unit	Source
hf	40.66	kJ/mol	Joback Method
hvap	81.94	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.785		Crippen Method
mcvol	238.490	ml/mol	McGowan Method
pc	1913.58	kPa	Joback Method
rinpol	2332.00		NIST Webbook
rinpol	2332.00		NIST Webbook
tb	845.34	K	Joback Method
tc	1068.98	K	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=U407550&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

hf:	Enthalpy of formation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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