

Urea, N,N-diphenyl-N'-hexyl-

Inchi:	InChI=1S/C19H24N2O/c1-2-3-4-11-16-20-19(22)21(17-12-7-5-8-13-17)18-14-9-6-10-15-
InchiKey:	KLSMWXFMMNUXAM-UHFFFAOYSA-N
Formula:	C19H24N2O
SMILES:	CCCCCN=C(O)N(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	296.41

Physical Properties

Property code	Value	Unit	Source
hf	25.30	kJ/mol	Joback Method
hvap	84.56	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	5.319		Crippen Method
mcvol	252.580	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	2485.00		NIST Webbook
rinpol	2485.00		NIST Webbook
tb	868.66	K	Joback Method
tc	1087.79	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=U407553&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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