

Urea, N,N-diphenyl-N'-octyl-

Inchi:	InChI=1S/C21H28N2O/c1-2-3-4-5-6-13-18-22-21(24)23(19-14-9-7-10-15-19)20-16-11-8-
InchiKey:	KUCLHJRQRGSKFN-UHFFFAOYSA-N
Formula:	C21H28N2O
SMILES:	CCCCCCCCN=C(O)N(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	324.46

Physical Properties

Property code	Value	Unit	Source
hf	-15.98	kJ/mol	Joback Method
hvap	89.01	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	6.099		Crippen Method
mcvol	280.760	ml/mol	McGowan Method
pc	1499.99	kPa	Joback Method
rinpol	2689.00		NIST Webbook
rinpol	2689.00		NIST Webbook
tb	914.42	K	Joback Method
tc	1132.63	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=U407556&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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