

Urea, N,N-diphenyl-N'-heptyl-

Inchi:	InChI=1S/C20H26N2O/c1-2-3-4-5-12-17-21-20(23)22(18-13-8-6-9-14-18)19-15-10-7-11-
InchiKey:	WBTOJSPEHOJXOG-UHFFFAOYSA-N
Formula:	C20H26N2O
SMILES:	CCCCCCN=C(O)N(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	310.43

Physical Properties

Property code	Value	Unit	Source
hf	4.66	kJ/mol	Joback Method
hvap	86.78	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	5.709		Crippen Method
mcvol	266.670	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	2586.00		NIST Webbook
rinpol	2586.00		NIST Webbook
tb	891.54	K	Joback Method
tc	1109.84	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407555&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

Latest version available from:

<https://www.cheméo.com/cid/96-442-5/Urea-N-N-diphenyl-N-heptyl.pdf>

Generated by Cheméo on 2024-04-26 05:50:27.180318539 +0000 UTC m=+16399876.100895854.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.