Methyldymron

Other names: Urea, N-methyl-N'-(1-methyl-1-phenylethyl)-N-phenyl-
Inchi: InChI=1S/C18H22N2O/c1-14-10-12-16(13-11-14)20(4)17(21)19-18(2,3)15-8-6-5-7-9-15/h
InchiKey: PQLUFUDWFGZVEG-UHFFFAOYSA-N
Formula: C18H22N2O
SMILES: Cc1ccc(N(C)C(O)=NC(C)(C)c2ccccc2)cc1
Mol. weight [g/mol]: 282.38
CAS: 42609-73-4

Physical Properties

Property code	Value	Unit	Source
hf	25.72	kJ/mol	Joback Method
hvap	81.70	kJ/mol	Joback Method
log10ws	-3.35		Aqueous Solubility Prediction Method
log10ws	-3.35		Estimated Solubility Method
logp	4.281		Crippen Method
mcvol	238.490	ml/mol	McGowan Method
pc	1906.90	kPa	Joback Method
rinpol	2062.00		NIST Webbook
tb	847.53	K	Joback Method
tc	1077.79	K	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C42609734&Units=SI

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