

Urea, 1-(2',4'-di-tert-butylphenyl)-3,3-diethyl-

Inchi: InChI=1S/C19H32N2O/c1-9-21(10-2)17(22)20-16-12-11-14(18(3,4)5)13-15(16)19(6,7)8/H
InchiKey: AJGLAMQKVBDIEA-UHFFFAOYSA-N
Formula: C19H32N2O
SMILES: CCN(CC)C(O)=Nc1ccc(C(C)(C)C)cc1C(C)(C)C
Mol. weight [g/mol]: 304.47

Physical Properties

Property code	Value	Unit	Source
hf	-251.67	kJ/mol	Joback Method
hvap	81.01	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	5.169		Crippen Method
mcvol	276.340	ml/mol	McGowan Method
pc	1358.63	kPa	Joback Method
tb	845.48	K	Joback Method
tc	1054.57	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=B6009302&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature

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