

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

**Inchi:** InChI=1S/C18H30N2O/c1-12(2)19-16(21)20-15-10-9-13(17(3,4)5)11-14(15)18(6,7)8/h9-18  
**InchiKey:** JXEQUBFSUKRCTN-UHFFFAOYSA-N  
**Formula:** C18H30N2O  
**SMILES:** CC(C)N=C(O)Nc1ccc(C(C)(C)C)cc1C(C)(C)C  
**Mol. weight [g/mol]:** 290.44

## Physical Properties

Property code	Value	Unit	Source
hf	-250.37	kJ/mol	Joback Method
hvap	82.79	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	5.016		Crippen Method
mcvol	262.250	ml/mol	McGowan Method
pc	1486.14	kPa	Joback Method
tb	859.89	K	Joback Method
tc	1075.55	K	Joback Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009303&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## 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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