

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

Inchi:	InChI=1S/C17H28N2O/c1-16(2,3)12-9-10-14(18-15(20)19(7)8)13(11-12)17(4,5)6/h9-11H
InchiKey:	VXHVOZOVOKRODX-UHFFFAOYSA-N
Formula:	C17H28N2O
SMILES:	CN(C)C(=O)Nc1ccc(C(C)(C)C)cc1C(C)(C)C
Mol. weight [g/mol]:	276.42

Physical Properties

Property code	Value	Unit	Source
gf	262.34	kJ/mol	Joback Method
hf	-189.70	kJ/mol	Joback Method
hfus	27.94	kJ/mol	Joback Method
hvap	69.67	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	4.375		Crippen Method
mcvol	248.160	ml/mol	McGowan Method
pc	1683.79	kPa	Joback Method
tb	735.02	K	Joback Method
tc	948.38	K	Joback Method
tf	472.71	K	Joback Method
vc	0.916	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.54	J/molxK	735.02	Joback Method
cpg	747.51	J/molxK	770.58	Joback Method
cpg	764.28	J/molxK	806.14	Joback Method
cpg	779.94	J/molxK	841.70	Joback Method
cpg	794.59	J/molxK	877.26	Joback Method
cpg	808.31	J/molxK	912.82	Joback Method
cpg	821.20	J/molxK	948.38	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=B6009301&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume

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