Pyridine, 2,4,6-tris(1,1-dimethylethyl)-

Other names:	Pyridine, 2,4,6-tri-tert-butyl-
	2,4,6-Tri-tert-butylpyridine
	2,4,6-Tri(t-butyl)pyridine
Inchi:	InChI=1S/C17H29N/c1-15(2,3)12-10-13(16(4,5)6)18-14(11-12)17(7,8)9/h10-11H,1-9H3
InchiKey:	IDOFMGSESVXXQI-UHFFFAOYSA-N
Formula:	C17H29N
SMILES:	CC(C)(C)c1cc(C(C)(C)C)nc(C(C)(C)C)c1
Mol. weight [g/mol]:	247.42
CAS:	20336-15-6

Physical Properties

Property code	Value	Unit	Source
ie	8.60	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
log10ws	-5.18		Crippen Method
logp	4.974		Crippen Method
mcvol	236.610	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20336156&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume