1H-Benzimidazole, 2-(1,1-dimethylethyl)-

Other names:	Benzimidazole, 2-tert-butyl-
	2-tert-Butylbenzimidazole
	2-(1,1-dimethylethyl)-1H-benzimidazole
Inchi:	InChI=1S/C11H14N2/c1-11(2,3)10-12-8-6-4-5-7-9(8)13-10/h4-7H,1-3H3,(H,12,13)
InchiKey:	ZQWHWRQRGKZTSE-UHFFFAOYSA-N
Formula:	C11H14N2
SMILES:	CC(C)(C)c1nc2ccccc2[nH]1
Mol. weight [g/mol]:	174.24
CAS:	24425-13-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	2.378		Crippen Method
mcvol	146.890	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=C24425136&Units=SI

Legend

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