

Benzimidazole, 2-(1,1,3-trimethylbutyl)-

Inchi:	InChI=1S/C14H20N2/c1-10(2)9-14(3,4)13-15-11-7-5-6-8-12(11)16-13/h5-8,10H,9H2,1-4H
InchiKey:	VXJPGFYLJDQASY-UHFFFAOYSA-N
Formula:	C14H20N2
SMILES:	CC(C)CC(C)(C)c1nc2ccccc2[nH]1
Mol. weight [g/mol]:	216.32
CAS:	116465-69-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.59		Crippen Method
logp	3.405		Crippen Method
mcvol	189.160	ml/mol	McGowan Method

Sources

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=C116465691&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/51-260-6/Benzimidazole-2-1-1-3-trimethylbutyl.pdf>

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