

1H-Benzotriazole, 1-(phenylmethyl)-

Other names:	1H-Benzotriazole, 1-benzyl- 1-Benzylbenzotriazole 1-Benzyl-1,2,3-benzotriazole 1-Benzyl-1H-benzotriazole
Inchi:	InChI=1S/C13H11N3/c1-2-6-11(7-3-1)10-16-13-9-5-4-8-12(13)14-15-16/h1-9H,10H2
InchiKey:	OQVSPZZIBWDHOF-UHFFFAOYSA-N
Formula:	C13H11N3
SMILES:	<chem>c1ccc(Cn2nnc3ccccc32)cc1</chem>
Mol. weight [g/mol]:	209.25
CAS:	4706-43-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.37		Crippen Method
logp	2.480		Crippen Method
mcvol	161.290	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=C4706438&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

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