1H-Benzotriazole, 1-phenyl-

Other names:	1-Phenyl-1,2,3-benzotriazole
	1-Phenylbenzotriazole
Inchi:	InChI=1S/C12H9N3/c1-2-6-10(7-3-1)15-12-9-5-4-8-11(12)13-14-15/h1-9H
InchiKey:	ZBJLUVHQIPUCPM-UHFFFAOYSA-N
Formula:	C12H9N3
SMILES:	c1ccc(-n2nnc3ccccc32)cc1
Mol. weight [g/mol]:	195.22
CAS:	883-39-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.46		Crippen Method
logp	2.420		Crippen Method
mcvol	147.200	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=C883396&Units=SI

Legend

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

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