

Imidazole-5-carboxylic acid, 1-benzyl-, methyl ester

Other names:	methyl 1-benzyl-1H-imidazole-5-carboxylate
Inchi:	InChI=1S/C12H12N2O2/c1-16-12(15)11-7-13-9-14(11)8-10-5-3-2-4-6-10/h2-7,9H,8H2,1H
InchiKey:	DOTNQIPIURWNFJ-UHFFFAOYSA-N
Formula:	C12H12N2O2
SMILES:	COC(=O)c1cncn1Cc1ccccc1
Mol. weight [g/mol]:	216.24
CAS:	73941-33-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.04		Crippen Method
logp	1.718		Crippen Method
mcvol	164.120	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=C73941330&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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