

1H-Imidazole-2-carboxaldehyde, 1-(phenylmethyl)-

Other names:	Imidazole-2-carboxaldehyde, 1-benzyl- 1-Benzyl-2-formylimidazole 1-Benzylimidazole-2-carboxaldehyde
Inchi:	InChI=1S/C11H10N2O/c14-9-11-12-6-7-13(11)8-10-4-2-1-3-5-10/h1-7,9H,8H2
InchiKey:	AKFHFMMKMUJLBU-UHFFFAOYSA-N
Formula:	C11H10N2O
SMILES:	O=Cc1nccn1Cc1ccccc1
Mol. weight [g/mol]:	186.21
CAS:	10045-65-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.04		Crippen Method
logp	1.744		Crippen Method
mcvol	144.160	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=C10045655&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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