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