Cyclopropanecarboxamide, n-benzimidazole-2-yl-

Inchi: InChI=1S/C11H11N3O/c15-10(7-5-6-7)14-11-12-8-3-1-2-4-9(8)13-11/h1-4,7H,5-6H2,(H2

InchiKey: COCUPSQZVJKBIO-UHFFFAOYSA-N

Formula: C11H11N3O

SMILES: OC(=Nc1nc2ccccc2[nH]1)C1CC1

Mol. weight [g/mol]: 201.22

CAS: 17228-32-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.14		Crippen Method
logp	2.079		Crippen Method
mcvol	147.580	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=C17228329&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume