Propionamide, n-(benzimidazol-2-yl)-2-methyl-

Inchi: InChI=1S/C11H13N3O/c1-7(2)10(15)14-11-12-8-5-3-4-6-9(8)13-11/h3-7H,1-2H3,(H2,12,
InchiKey: JVFBVPWDPRTTLQ-UHFFFAOYSA-N
Formula: C11H13N3O
SMILES: CC(C)C(O)=Nc1nc2ccccc2[nH]1
Mol. weight [g/mol]: 203.24
CAS: 17228-23-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.24		Crippen Method
logp	2.325		Crippen Method
mcvol	158.440	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=C17228238&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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