

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/ci9903071

Legend

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

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<https://www.chemeo.com/cid/86-109-6/Propionamide-n-benzimidazol-2-yl-2-methyl.pdf>

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