Propenoic acid, 3-(1-methyl-2-benzimidazolyl)-

Inchi: InChI=1S/C11H10N2O2/c1-13-9-5-3-2-4-8(9)12-10(13)6-7-11(14)15/h2-7H,1H3,(H,14,15
InchiKey: MFJCQRHGLKEFEG-VOTSOKGWSA-N
Formula: C11H10N2O2
SMILES: Cn1c(C=CC(=O)O)nc2ccccc21
Mol. weight [g/mol]: 202.21
CAS: 30769-96-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.67		Crippen Method
logp	1.671		Crippen Method
mcvol	150.030	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=C30769961&Units=SI

Legend

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