1-Isopropenyl-2-benzimidazolinone

Other names: 1,3-dihydro-1-(1-methylvinyl)-2H-benzimidazol-2-one
Inchi: InChI=1S/C10H10N2O/c1-7(2)12-9-6-4-3-5-8(9)11-10(12)13/h3-6H,1H2,2H3,(H,11,13)
InchiKey: XFASJWLBXHWUMW-UHFFFAOYSA-N
Formula: C10H10N2O
SMILES: C=C(C)n1c(O)nc2ccccc21
Mol. weight [g/mol]: 174.20
CAS: 52099-72-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.29		Crippen Method
logp	2.232		Crippen Method
mcvol	134.370	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=C52099726&Units=SI

Legend

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