

2-Methoxy-1-methyl-4-quinolone

Inchi: InChI=1S/C11H11NO2/c1-12-9-6-4-3-5-8(9)10(13)7-11(12)14-2/h3-7H,1-2H3
InchiKey: RMPAXAAOZFGZSS-UHFFFAOYSA-N
Formula: C11H11NO2
SMILES: COc1cc(=O)c2ccccc2n1C
Mol. weight [g/mol]: 189.21
CAS: 40335-01-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.11		Crippen Method
logp	1.547		Crippen Method
mcvol	144.350	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C40335011&Units=SI>
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>

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/64-912-8/2-Methoxy-1-methyl-4-quinolone.pdf>

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