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

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=C40335011&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

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