

1-Hydroxy-3-methoxyacridin-9(10H)-one

Inchi: InChI=1S/C14H11NO3/c1-18-8-6-11-13(12(16)7-8)14(17)9-4-2-3-5-10(9)15-11/h2-7,16H
InchiKey: LJHHYEQRALVSL-LUHFFFAOYSA-N
Formula: C₁₄H₁₁NO₃
SMILES: COc1cc(O)c2c(=O)c3ccccc3[nH]c2c1
Mol. weight [g/mol]: 241.24
CAS: 91998-87-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.39		Crippen Method
logp	1.914		Crippen Method
mcvol	173.030	ml/mol	McGowan Method
rmpol	2806.80		NIST Webbook
rmpol	2806.80		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemo.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=C91998877&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rmpol: Non-polar retention indices

Latest version available from:

<https://www.chemo.com/cid/116-101-0/1-Hydroxy-3-methoxyacridin-9-10H-one.pdf>

Generated by Cheméo on 2024-05-03 04:53:47.120061344 +0000 UTC m=+17001276.040638660.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.