

9(10H)-Acridinone, 1-hydroxy-3-methoxy-10-methyl-

Other names: 9-Acridanone, 1-hydroxy-3-methoxy-10-methyl-
1-Hydroxy-3-methoxy-N-methylacridone

Inchi: InChI=1S/C15H13NO3/c1-16-11-6-4-3-5-10(11)15(18)14-12(16)7-9(19-2)8-13(14)17/h3-

InchiKey: OCUBFJMZYIVBO-UHFFFAOYSA-N

Formula: C15H13NO3

SMILES: COc1cc(O)c2c(=O)c3ccccc3n(C)c2c1

Mol. weight [g/mol]: 255.27

CAS: 13161-83-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.46		Crippen Method
logp	2.406		Crippen Method
mcvol	187.120	ml/mol	McGowan Method
rinpol	2825.90		NIST Webbook
rinpol	2825.90		NIST Webbook

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=C13161836&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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