

1-Hydroxy-3,4-dimethoxy-10-methylacridin-9(10H)

Inchi: InChI=1S/C16H15NO4/c1-17-10-7-5-4-6-9(10)15(19)13-11(18)8-12(20-2)16(21-3)14(13)
InchiKey: FPTMTPTVCVDIMW-UHFFFAOYSA-N
Formula: C16H15NO4
SMILES: COc1cc(O)c2c(=O)c3ccccc3n(C)c2c1OC
Mol. weight [g/mol]: 285.29
CAS: 96935-29-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.58		Crippen Method
logp	2.414		Crippen Method
mcvol	207.080	ml/mol	McGowan Method
rinpol	2785.60		NIST Webbook
rinpol	2785.60		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C96935294&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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