

1,3-Dioxolo[4,5-c]acridin-6(11H)-one, 4,5-dimethoxy-11-methyl-

Other names:

Melicopine

4,5-dimethoxy-11-methyl-1,3-dioxolo[4,5-c]acridin-6(11H)-one

Inchi:

InChI=1S/C17H15NO5/c1-18-10-7-5-4-6-9(10)13(19)11-12(18)15-17(23-8-22-15)16(21-3

InchiKey:

PEWWLIQAXYMMAN-UHFFFAOYSA-N

Formula:

C17H15NO5

SMILES:

COc1c2c(c3c(c1OC)c(=O)c1cccc1n3C)OCO2

Mol. weight [g/mol]:

313.30

CAS:

568-01-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.24		Crippen Method
logp	2.438		Crippen Method
mcvol	216.180	ml/mol	McGowan Method
rinpol	3000.00		NIST Webbook
rinpol	3000.00		NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=C568014&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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