

1,3-Dioxolo[4,5-b]acridin-10(5H)-one, 4,11-dimethoxy-5-methyl-

Other names:	Melicopidine Melicopidene 4,11-Dimethoxy-5-methyl-1,3-dioxolo(4,5-b)acridin-10(5H)-one
Inchi:	InChI=1S/C17H15NO5/c1-18-10-7-5-4-6-9(10)13(19)11-12(18)15(21-3)17-16(14(11)20-2
InchiKey:	TZZNUDMEMFBPQI-UHFFFAOYSA-N
Formula:	C17H15NO5
SMILES:	COc1c2c(c(OC)c3c1c(=O)c1cccc1n3C)OCO2
Mol. weight [g/mol]:	313.30
CAS:	475-91-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.24		Crippen Method
logp	2.438		Crippen Method
mcvol	216.180	ml/mol	McGowan Method
rropol	2955.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C475912&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rropol:	Non-polar retention indices

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