

Acronine

Other names:	7H-Pyrano[2,3-c]acridin-7-one, 3,12-dihydro-6-methoxy-3,3,12-trimethyl-Acrorycine Acromycine Compound 42339 NCI-C01536 NSC 403169 3,12-Dihydro-6-methoxy-3,3,12-trimethyl-7H-pyrano(2,3-c)acridin-7-one 42339 6-Methoxy-3,3,12-trimethyl-3,12-dihydro-7H-pyrano[2,3-c]acridin-7-one
Inchi:	InChI=1S/C20H19NO3/c1-20(2)10-9-13-15(24-20)11-16(23-4)17-18(13)21(3)14-8-6-5-7-
InchiKey:	SMPZPKRDRQOOHT-UHFFFAOYSA-N
Formula:	C20H19NO3
SMILES:	<chem>COc1cc2c(c3c1c(=O)c1cccc1n3C)C=CC(C)(C)O2</chem>
Mol. weight [g/mol]:	321.37
CAS:	7008-42-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.70		Crippen Method
logp	3.884		Crippen Method
mcvol	242.410	ml/mol	McGowan Method

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=C7008426&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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