Furo[2,3-c]acridin-6(2H)-one, 1,11-dihydro-5-hydroxy-11-methyl-2-(1-methyleth (-)-

Other names: Rutacridone
InChI: InChI=1S/C19H17NO3/c1-10(2)15-8-12-16(23-15)9-14(21)17-18(12)20(3)13-7-5-4-6-11(
InchiKey: FHAGACMCMQYSNX-UHFFFAOYSA-N
Formula: C19H17NO3
SMILES: C=C(C)C1Cc2c(cc(O)c3c(=O)c4ccccc4n(C)c23)O1
Mol. weight [g/mol]: 307.34
CAS: 17948-33-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.96		Crippen Method
logp	3.277		Crippen Method
mcvol	228.320	ml/mol	McGowan Method
rinpol	3258.00		NIST Webbook
rinpol	3258.00		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=C17948333&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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