

Swerchirin

Inchi: InChI=1S/C15H12O6/c1-19-7-5-9(17)12-11(6-7)21-15-10(20-2)4-3-8(16)13(15)14(12)18/
InchiKey: GNSHHHWDGOHNPC-UHFFFAOYSA-N
Formula: C15H12O6
SMILES: COc1cc(O)c2c(=O)c3c(O)ccc(OC)c3oc2c1
Mol. weight [g/mol]: 288.25
CAS: 521-65-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.57		Crippen Method
logp	2.375		Crippen Method
mcvol	194.750	ml/mol	McGowan Method
rinpol	2625.50		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=C521653&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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<https://www.chemeo.com/cid/75-226-8/Swerchirin.pdf>

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