

Doronanine

Inchi: InChI=1S/C18H25NO5/c1-11-8-12(2)18(3,22)17(21)23-10-14-5-4-13-6-7-15(19(13)14)24
InchiKey: SBROHHBIDHUOIN-LUAWRHEFSA-N
Formula: C18H25NO5
SMILES: CC1=CC(=O)OC2CCC3CC=C(COC(=O)C(C)(O)C(C)C1)N32
Mol. weight [g/mol]: 335.39
CAS: 74217-57-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.39		Crippen Method
logp	1.888		Crippen Method
mcvol	254.030	ml/mol	McGowan Method
rinpola	2335.00		NIST Webbook

Sources

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=C74217575&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

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<https://www.chemeo.com/cid/99-534-0/Doronanine.pdf>

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