

Jacozine

Inchi: InChI=1S/C18H23NO6/c1-10-8-18(11(2)25-18)16(21)24-13-5-7-19-6-4-12(14(13)19)9-23
InchiKey: XCEPKQNOWNOSFH-UHFFFAOYSA-N
Formula: C18H23NO6
SMILES: C=C1CC2(OC2C)C(=O)OC2CCN3CC=C(COC(=O)C1(C)O)C23
Mol. weight [g/mol]: 349.38
CAS: 5532-23-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.85		Crippen Method
logp	0.324		Crippen Method
mcvol	249.040	ml/mol	McGowan Method
rinpol	2460.00		NIST Webbook
rinpol	2466.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5532230&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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
rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/69-064-5/Jacozine.pdf>

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