

7,9-Diseneciolyheliotridine

Inchi: InChI=1S/C18H25NO4/c1-12(2)9-16(20)22-11-14-5-7-19-8-6-15(18(14)19)23-17(21)10-1
InchiKey: HYBMOCMONQPISM-QAPCUYQASA-N
Formula: C18H25NO4
SMILES: CC(C)=CC(=O)OCC1=CCN2CCC(OC(=O)C=C(C)C)C12
Mol. weight [g/mol]: 319.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.23		Crippen Method
logp	2.388		Crippen Method
mcvol	254.720	ml/mol	McGowan Method
rinpol	2275.00		NIST Webbook
rinpol	2277.00		NIST Webbook
rinpol	2325.00		NIST Webbook
rinpol	2275.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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=R522348&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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