

7,9-Ditigloylheliotridine

Inchi: InChI=1S/C18H25NO4/c1-5-12(3)17(20)22-11-14-7-9-19-10-8-15(16(14)19)23-18(21)13
InchiKey: HMXNAWUWVBSLJC-UITJNDFPSA-N
Formula: C18H25NO4
SMILES: CC=C(C)C(=O)OCC1=CCN2CCC(OC(=O)C(C)=CC)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
rinpole	2275.00		NIST Webbook
rinpole	2276.00		NIST Webbook
rinpole	2325.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R177790&Units=SI>
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>

Legend

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

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<https://www.chemeo.com/cid/12-322-0/7-9-Ditigloylheliotridine.pdf>

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