

9-curassavoylheliotridine

Inchi: InChI=1S/C16H27NO5/c1-4-10(2)16(21,11(3)18)15(20)22-9-12-5-7-17-8-6-13(19)14(12)
InchiKey: JEACDFMOGUTDGW-LBVNJDACSA-N
Formula: C16H27NO5
SMILES: CCC(C)C(O)(C(=O)OCC1=CCN2CCC(O)C12)C(C)O
Mol. weight [g/mol]: 313.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.59		Crippen Method
logp	0.063		Crippen Method
mcvol	245.310	ml/mol	McGowan Method
rinpol	2190.00		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=R227944&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

Latest version available from:

<https://www.chemeo.com/cid/14-938-5/9-curassavoylheliotridine.pdf>

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