7-Senecioylheliotridine

Inchi: InChI=1S/C13H19NO3/c1-9(2)7-12(16)17-11-4-6-14-5-3-10(8-15)13(11)14/h3,7,11,13,15
InchiKey: JWVMHVYNWULPCC-YPMHNXCESA-N
Formula: C13H19NO3
SMILES: CC(C)=CC(=O)OC1CCN2CC=C(CO)C12
Mol. weight [g/mol]: 237.29
CAS: 146450-65-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.68		Crippen Method
logp	0.871		Crippen Method
mcvol	187.000	ml/mol	McGowan Method
rinpol	1868.00		NIST Webbook
rinpol	1868.00		NIST Webbook
rinpol	1915.00		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=C146450659&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
rinpol: Non-polar retention indices

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