

3«alpha»-Seneciolyloxytropane

Inchi: InChI=1S/C13H21NO2/c1-9(2)6-13(15)16-12-7-10-4-5-11(8-12)14(10)3/h6,10-12H,4-5,7
InchiKey: PFQFRMFXPJMNJJ-GDNZZTSVSA-N
Formula: C13H21NO2
SMILES: CC(C)=CC(=O)OC1CC2CCC(C1)N2C
Mol. weight [g/mol]: 223.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.68		Crippen Method
logp	2.121		Crippen Method
mcvol	185.430	ml/mol	McGowan Method
rinpol	1659.00		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1661.00		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=R570104&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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