6-Hydroxyapoatropine

Inchi: InChI=1S/C17H21NO3/c1-11(12-6-4-3-5-7-12)17(20)21-14-8-13-9-16(19)15(10-14)18(13
InchiKey: IZVZMPYXRCTCEG-UHFFFAOYSA-N
Formula: C17H21NO3
SMILES: C=C(C(=O)OC1CC2CC(O)C(C1)N2C)c1ccccc1
Mol. weight [g/mol]: 287.35
CAS: 131899-21-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.00		Crippen Method
logp	1.839		Crippen Method
mcvol	223.900	ml/mol	McGowan Method
rinpol	2306.30		NIST Webbook
rinpol	2306.30		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=C131899213&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