Aposcopolamine

Inchi: InChI=1S/C17H19NO3/c1-10(11-6-4-3-5-7-11)17(19)20-12-8-13-15-16(21-15)14(9-12)18
InchiKey: JJNVDCBKBUSUII-UHFFFAOYSA-N
Formula: C17H19NO3
SMILES: C=C(C(=O)OC1CC2C3OC3C(C1)N2C)c1ccccc1
Mol. weight [g/mol]: 285.34
CAS: 535-26-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.83		Crippen Method
logp	1.855		Crippen Method
mcvol	213.040	ml/mol	McGowan Method
rinpol	2223.50		NIST Webbook
rinpol	2223.50		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=C535262&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