Methylscopolamine

Inchi: InChI=1S/C17H21NO4/c1-18-13-7-11(8-14(18)16-15(13)22-16)21-17(20)12(9-19)10-5-3-
InchiKey: STECJAGHUSJQJN-SDODBCEQSA-N
Formula: C17H21NO4
SMILES: CN1C2CC(OC(=O)C(CO)c3ccccc3)CC1C1OC12
Mol. weight [g/mol]: 303.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.03		Crippen Method
logp	0.918		Crippen Method
mcvol	223.210	ml/mol	McGowan Method
rinpol	2172.00		NIST Webbook
rinpol	2172.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R421780&Units=SI
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

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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