3-Hydroxy-2-phenyl-propionic acid 6-hydroxy-8-methyl-8-aza-bicyclo[3.2.1]oct-3-yl ester

Othernames: 7-Hydroxyhyoscyamine
7«beta»-Hydroxyhyoscyamine
Inchi: InChI=1S/C17H23NO4/c1-18-12-7-13(9-15(18)16(20)8-12)22-17(21)14(10-19)11-5-3-2-4
InchiKey: WTQYWNWRJNXDEG-UHFFFAOYSA-N
Formula: C17H23NO4
SMILES: CN1C2CC(OC(=O)C(CO)c3ccccc3)CC1C(O)C2
Mol. weight [g/mol]: 305.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.20		Crippen Method
logp	0.902		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
rinpol	2332.00		NIST Webbook
rinpol	2335.00		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=U301241&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

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