

6«beta»-Hydroxyhyoscyamine

Other names:	6-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-BLJPBYAASA-N
Formula:	C17H23NO4
SMILES:	CN1C2CC(OC(=O)C(CO)c3ccccc3)CC1C(O)C2
Mol. weight [g/mol]:	305.37
CAS:	52646-91-0

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	2308.00		NIST Webbook
rinpol	2355.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52646910&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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