Homatropine

Other names:	Benzeneacetic acid, «alpha»-hydroxy-, 8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, endo-(.+/-.)-
	1«alpha»H,5«alpha»H-Tropan-3-«alpha»-ol, mandelate
	Homatropin
	Homoatropine
	Homotropine
	Mandelic acid, 3d-tropanyl ester
	Mandelyltropeine
	Mandelytropeine
	Tropine, mandelate
	3«alpha»-Hydroxy-1«alpha»H,5«alpha»H-tropanium mandelate (ester)
	(.+/-.)-Homatropine
Inchi:	InChI=1S/C16H21NO3/c1-17-12-7-8-13(17)10-14(9-12)20-16(19)15(18)11-5-3-2-4-6-11/h
InchiKey:	ZTVIKZXZYLEVOL-UHFFFAOYSA-N
Formula:	C16H21NO3
SMILES:	CN1C2CCC1CC(OC(=O)C(O)c1ccccc1)C2
Mol. weight [g/mol]:	275.34
CAS:	87-00-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.90		Crippen Method
logp	1.888		Crippen Method
mcvol	214.110	ml/mol	McGowan Method
rinpol	2095.00		NIST Webbook
rinpol	2072.00		NIST Webbook
rinpol	2072.00		NIST Webbook
rinpol	2070.00		NIST Webbook
rinpol	2095.00		NIST Webbook
rinpol	2070.00		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=C87003&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