Benzeneacetic acid, «alpha»-methylene-, 8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, endo-

Other names:	1-«alpha»-H,5-«alpha»-H-Tropan-3-«alpha»-ol, atropate Apoatropin Apoatropine Atropamin Atropamine Atropyltropeine endo-«alpha»-Methylenebenzeneacetic acid 8-methyl-8-azabicyclo(3.2.1)oct-3-yl ester Tropic acid, 3-«alpha»-tropanyl ester Tropine, atropate Apohyoscyamin Apohyoscyamine Benzeneacetic acid, «alpha»-methylene-, (3-endo)-8-methyl-8-azabicyclo(3.2.1)oct-3-yl ester 1-«alpha»-5H«alpha»-Tropan-3«alpha»-ol, atropate (ester)
Inchi:	InChI=1S/C17H21NO2/c1-12(13-6-4-3-5-7-13)17(19)20-16-10-14-8-9-15(11-16)18(14)2/h
InchiKey:	WPUIZWXOSDVQJU-UHFFFAOYSA-N
Formula:	C17H21NO2
SMILES:	C=C(C(=O)OC1CC2CCC(C1)N2C)c1ccccc1
Mol. weight [g/mol]:	271.35
CAS:	500-55-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.62		Crippen Method
logp	2.868		Crippen Method
mcvol	218.030	ml/mol	McGowan Method
rinpol	2105.30		NIST Webbook
rinpol	2028.00		NIST Webbook
rinpol	2050.00		NIST Webbook
rinpol	2028.00		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=C500550&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