Tropacocaine

Other names:	8-Azabicyclo[3.2.1]octan-3-ol, 8-methyl-, benzoate, exo- 1«alpha»-H,5«alpha»-H-Tropan-3«beta»-ol, benzoate Benzilate of pseudotropanol Benzoylpseudotropeine Benzoylpseudotropine Benzoyl-psi-tropeine o-Benzoyltropine exo-8-Methyl-8-azabicyclo(3.2.1)-octan-3-ol benzoate Pseudotropanol benzilate Pseudotropine benzoate Tropacaine Tropacocain psi-Tropine benzoate 8-Azabicyclo[3.2.1]octan-3-ol, 8-methyl-, benzoate (ester), exo- «psi»-Tropine benzoate Pseudotropine, benzoate (ester)
Inchi:	InChI=1S/C15H19NO2/c1-16-12-7-8-13(16)10-14(9-12)18-15(17)11-5-3-2-4-6-11/h2-6,12
InchiKey:	XQJMXPAEFMWDOZ-UHFFFAOYSA-N
Formula:	C15H19NO2
SMILES:	CN1C2CCC1CC(OC(=O)c1ccccc1)C2
Mol. weight [g/mol]:	245.32
CAS:	537-26-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.34		Crippen Method
logp	2.469		Crippen Method
mcvol	194.150	ml/mol	McGowan Method
rinpol	1974.00		NIST Webbook
rinpol	1965.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1952.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1940.00		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=C537268&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