Clemastine

Other names: Pyrrolidine, 2-[2-[1-(4-chlorophenyl)-1-phenylethoxy]ethyl]-1-methyl-, [R-(R*,R*)]-
(+)-(2R)-2-[2-[[(R)-p-Chloro-«alpha»-methyl-«alpha»-phenylbenzyl]oxy]ethyl]-1-methylpyr
Meclastine
Inchi: InChI=1S/C21H26ClNO/c1-21(17-7-4-3-5-8-17,18-10-12-19(22)13-11-18)24-16-14-20-9-
InchiKey: YNNUSGIPVFPVBX-UHFFFAOYSA-N
Formula: C21H26ClNO
SMILES: CN1CCCC1CCOC(C)(c1ccccc1)c1ccc(Cl)cc1
Mol. weight [g/mol]: 343.89
CAS: 15686-51-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.44		Crippen Method
logp	5.104		Crippen Method
mcvol	276.460	ml/mol	McGowan Method
rinpol	2430.00		NIST Webbook
rinpol	2415.00		NIST Webbook
rinpol	2420.00		NIST Webbook
rinpol	2420.00		NIST Webbook
rinpol	2446.00		NIST Webbook
rinpol	2420.00		NIST Webbook

Sources

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=C15686518&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices