Benztropine

Other names:	8-Azabicyclo[3.2.1]octane, 3-(diphenylmethoxy)-8-methyl-, endo- 1«alpha»H,5«alpha»H-Tropane, 3«alpha»-(diphenylmethoxy)- Akitan Benzotropine Cobrentin Cogentinol NK-02 Tropine benzohydryl ether Cogentine 3«alpha»-(Diphenylmethoxy)-1«alpha»H,5«alpha»H-tropane 8-Azabicyclo[3.2.1]octane, 3-(diphenylmethoxy)-8-methyl-, (3-endo)- Benzatropine
Inchi:	InChI=1S/C21H25NO/c1-22-18-12-13-19(22)15-20(14-18)23-21(16-8-4-2-5-9-16)17-10-6
InchiKey:	GIJXKZJWITVLHI-UHFFFAOYSA-N
Formula:	C21H25NO
SMILES:	CN1C2CCC1CC(OC(c1ccccc1)c1ccccc1)C2
Mol. weight [g/mol]:	307.43
CAS:	86-13-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.16		Crippen Method
logp	4.418		Crippen Method
mcvol	253.360	ml/mol	McGowan Method
rinpol	2310.00		NIST Webbook
rinpol	2334.00		NIST Webbook
rinpol	2320.00		NIST Webbook
rinpol	2287.00		NIST Webbook
rinpol	2314.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2302.00		NIST Webbook
rinpol	2287.00		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=C86135&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