Trihexyphenidyl

Other names:	1-Piperidinepropanol, «alpha»-cyclohexyl-«alpha»-phenyl-
	1-Piperidinepropanol, Â«alphaÂ»-cyclohexyl-Â«alphaÂ»-phenyl-
	1-cyclohexyl-1-phenyl-3-piperidin-1-ylpropan-1-ol
	Benzhexol
	Parkinane retard
	Sedrena (free base)
	Trihexylphenidyl
	Trihexylphenidyle
	Trihexylphenizyl
	Triphenidyl
	«alpha»-Cyclohexyl-«alpha»-phenyl-1-piperidinepropanol
	Â«alphaÂ»-Cyclohexyl-Â«alphaÂ»-phenyl-1-piperidinepropanol
Inchi:	InChI=1S/C20H31NO/c22-20(18-10-4-1-5-11-18,19-12-6-2-7-13-19)14-17-21-15-8-3-9-1
InchiKey:	HWHLPVGTWGOCJO-UHFFFAOYSA-N
Formula:	C20H31NO
SMILES:	OC(CCN1CCCCC1)(c1ccccc1)C1CCCCC1
Mol. weight [g/mol]:	301.47
CAS:	144-11-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.81		Aqueous Solubility Prediction Method
logp	4.331		Crippen Method
mcvol	263.030	ml/mol	McGowan Method
rinpol	2226.00		NIST Webbook
rinpol	2236.00		NIST Webbook
rinpol	2233.00		NIST Webbook
rinpol	2211.00		NIST Webbook
rinpol	2260.00		NIST Webbook
tf	387.65	K	Aqueous Solubility Prediction Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C144116&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
tf:	Normal melting (fusion) point