

Etodroxizine

Other names:	Etodroxine
Inchi:	InChI=1S/C23H31ClN2O3/c24-22-8-6-21(7-9-22)23(20-4-2-1-3-5-20)26-12-10-25(11-13-
InchiKey:	VUFOCTSXHUWGPW-UHFFFAOYSA-N
Formula:	C23H31ClN2O3
SMILES:	OCCOCCOCCN1CCN(C(c2ccccc2)c2ccc(Cl)cc2)CC1
Mol. weight [g/mol]:	418.96
CAS:	17692-34-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.37		Crippen Method
logp	3.073		Crippen Method
mcvol	326.360	ml/mol	McGowan Method
rinpol	3180.00		NIST Webbook
rinpol	3175.00		NIST Webbook
rinpol	3175.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17692341&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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