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