Allobarbital perethylated

Other names: Allobarbital ethylated
Inchi: InChI=1S/C14H20N2O3/c1-5-9-14(10-6-2)11(17)15(7-3)13(19)16(8-4)12(14)18/h5-6H,1-
InchiKey: UUCXEOIZJOXKSI-UHFFFAOYSA-N
Formula: C14H20N2O3
SMILES: C=CCC1(CC=C)C(=O)N(CC)C(=O)N(CC)C1=O
Mol. weight [g/mol]: 264.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.49		Crippen Method
logp	1.956		Crippen Method
mcvol	213.330	ml/mol	McGowan Method
rinpol	1563.00		NIST Webbook
rinpol	1563.00		NIST Webbook
rinpol	1563.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1563.00		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=R108353&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