

Oxyphencyclimine

Other names: Benzeneacetic acid, «alpha»-cyclohexyl-«alpha»-hydroxy-,
(1,4,5,6-tetrahydro-1-methyl-2-pyrimidinyl)methyl ester
(1,4,5,6-Tetrahydro-1-methyl-2-pyrimidinyl)methyl
«alpha»-phenylcyclohexaneglycolate
Antulcus

Caridan

Naridan

Zamanil

Inchi: InChI=1S/C20H28N2O3/c1-22-14-8-13-21-18(22)15-25-19(23)20(24,16-9-4-2-5-10-16)17

InchiKey: DUDKAZCAISNGQN-UHFFFAOYSA-N

Formula: C20H28N2O3

SMILES: CN1CCCN=C1COC(=O)C(O)(c1ccccc1)C1CCCCC1

Mol. weight [g/mol]: 344.45

CAS: 125-53-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.37		Crippen Method
logp	2.732		Crippen Method
mcvol	276.150	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C125531&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

Latest version available from:

<https://www.chemeo.com/cid/114-934-8/Oxyphencyclimine.pdf>

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