

Dihexyverine

Other names: 2-Piperidinoethyl ester of bicyclohexyl-1-carboxylic acid
Inchi: InChI=1S/C20H35NO2/c22-19(23-17-16-21-14-8-3-9-15-21)20(12-6-2-7-13-20)18-10-4-1
InchiKey: MNSQDVCVWNXBFQ-UHFFFAOYSA-N
Formula: C20H35NO2
SMILES: O=C(OCCN1CCCCC1)C1(C2CCCCC2)CCCCC1
Mol. weight [g/mol]: 321.50
CAS: 561-77-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.83		Crippen Method
logp	4.546		Crippen Method
mcvol	277.500	ml/mol	McGowan Method
rinpola	2315.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C561773&Units=SI>
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>

Legend

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

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