

Mepivacaine

Other names:	(.+/-)-1-Methyl-2',6'-piperidylidide (.+/-)-Mepivacaine 1-Methyl-2',6'-piperidylidide 2',6'-Piperidylidide, 1-methyl- 2-Piperidinecarboxamide, N-(2,6-dimethylphenyl)-1-methyl- Carbocain Carbocaine DL-Mepivacaine Mepivacaine N-(2,6-Dimethylphenyl)-1-methyl-2-piperidinecarboxamide N-(2,6-dimethylphenyl)-1-methylpiperidine-2-carboxamide N-Methyl-2-piperidic acid, 2,6-dimethylanilide N-Methyl-2-piperidic acid, 2,6-ylidide N-Methylhexahydro-2-picolinic acid, 2,6-dimethylanilide Scandicain Scandicaine Scandicane d,l-mepivacaine
Inchi:	InChI=1S/C15H22N2O/c1-11-7-6-8-12(2)14(11)16-15(18)13-9-4-5-10-17(13)3/h6-8,13H,
InchiKey:	INWLQCZOYSRPNW-UHFFFAOYSA-N
Formula:	C15H22N2O
SMILES:	<chem>Cc1ccc(C)c1NC(=O)C1CCCN1C</chem>
Mol. weight [g/mol]:	246.35
CAS:	96-88-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.55		Aqueous Solubility Prediction Method
logp	2.726		Crippen Method
mvol	209.120	ml/mol	McGowan Method
rinpol	2066.00		NIST Webbook
rinpol	2049.00		NIST Webbook
rinpol	2090.00		NIST Webbook
rinpol	2066.00		NIST Webbook
rinpol	2041.00		NIST Webbook
rinpol	2041.00		NIST Webbook

rmpol	2042.00		NIST Webbook
rmpol	2050.00		NIST Webbook
rmpol	2085.00		NIST Webbook
rmpol	2071.00		NIST Webbook
rmpol	2090.00		NIST Webbook
rmpol	2066.00		NIST Webbook
rmpol	2050.00		NIST Webbook
rmpol	2070.00		NIST Webbook
tf	423.65	K	Aqueous Solubility Prediction Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96888&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rmpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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