

Bupivacaine

Other names:	(. +/-)-1-Butyl-2',6'-pipercoloxylidide (. +/-)-Bupivacaine (±)-1-butyl-N-(2,6-dimethylphenyl)piperidine-2-carboxamide (∓)-1-butyl-N-(2,6-dimethylphenyl)piperidine-2-carboxamide 1-Butyl-2',6'-pipercoloxylidide 1-Butyl-N-(2,6-dimethylphenyl)-2-piperidinecarboxamide 2',6'-Pipercoloxylidide, 1-butyl- 2-Piperidinecarboxamide, 1-butyl-N-(2,6-dimethylphenyl)- 2-Piperidinecarboxamide, 1-butyl-N-(2,6-dimethylphenyl)-, (. +/-)- Anekain Carbostesin DL-Bupivacaine Marcaine Win 11318 bupibacaine dl-1-Butyl-2',6'-pipercoloxylidide
Inchi:	InChI=1S/C18H28N2O/c1-4-5-12-20-13-7-6-11-16(20)18(21)19-17-14(2)9-8-10-15(17)3/
InchiKey:	LEBVLXFERQHONN-UHFFFAOYSA-N
Formula:	C18H28N2O
SMILES:	CCCCN1CCCCC1C(O)=Nc1c(C)ccc1C
Mol. weight [g/mol]:	288.43
CAS:	38396-39-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.22		Aqueous Solubility Prediction Method
logp	4.546		Crippen Method
mcvol	251.390	ml/mol	McGowan Method
tf	370.65	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=C38396393&Units=SI>

Legend

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

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