

N-(2,6-dimethylphenyl)-1-methyl-2-piperidinecarb

Other names:	(.+/-.)-1-Methyl-2',6'-pipecoloxylidide (.+/-.)-Mepivacaine 1-Methyl-2',6'-pipecoloxylidide 2',6'-Pipecoloxylidide, 1-methyl- 2-Piperidinecarboxamide, N-(2,6-dimethylphenyl)-1-methyl- Carbocain Carbocaine DL-Mepivacaine Mepivacaine N-(2,6-dimethylphenyl)-1-methylpiperidine-2-carboxamide N-Methyl-2-pipecolic acid, 2,6-dimethylanilide N-Methyl-2-pipecolic acid, 2,6-xylidide 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:	Cc1cccc(C)c1NC(=O)C1CCCCN1C
Mol. weight [g/mol]:	246.35
CAS:	24358-84-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.55		Aqueous Solubility Prediction Method
logp	2.726		Crippen Method
mcvol	209.120	ml/mol	McGowan Method
tf	423.65	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	17.77	kJ/mol	426.20	NIST Webbook

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C24358847&Units=SI>

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

hfust: Enthalpy of fusion at a given temperature

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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