

Diphenoxylate

Other names:	1-(3-Cyano-3,3-diphenylpropyl)-4-phenyl-isonipecotic acid ethyl ester 1-(3-cyano-3,3-diphenylpropyl)-4-phenylisonipecotic acid ethyl ester 1-(3-cyano-3,3-diphenylpropyl)-4-phenylpiperidine-4-carboxylic acid ethyl ester 4-Piperidinecarboxylic acid, 1-(3-cyano-3,3-diphenylpropyl)-4-phenyl-, ethyl ester Diphenoxalate Ethyl-1-(3-cyano-3,3-diphenylpropyl)-4-phenylisonipecotate Isonipecotic acid, 1-(3-cyano-3,3-diphenylpropyl)-4-phenyl-, ethyl ester Lomotil R-1132 ethyl 1-(3-cyano-3,3-diphenylpropyl)-4-phenylpiperidine-4-carboxylate
Inchi:	InChI=1S/C30H32N2O2/c1-2-34-28(33)29(25-12-6-3-7-13-25)18-21-32(22-19-29)23-20-3
InchiKey:	HYPPXZBJBPSRLK-UHFFFAOYSA-N
Formula:	C30H32N2O2
SMILES:	CCOC(=O)C1(c2cccc2)CCN(CCC(C#N)(c2cccc2)c2cccc2)CC1
Mol. weight [g/mol]:	452.59
CAS:	915-30-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.33		Crippen Method
logp	5.483		Crippen Method
mcvol	370.220	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility and Solution Thermodynamics of Diphenoxylate in Different Pure Solvents:	https://www.doi.org/10.1021/je5010033
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C915300&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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