DIFENOXIN

Other names:	Isonipecotic acid, 1-(3-cyano-3,3-diphenylpropyl)-4-phenyl-
	Diphenoxin
	Difenoxine
	Diphenoxylic acid
	4-Piperidinecarboxylic acid, 1-(3-cyano-3,3-diphenylpropyl)-4-phenyl-
	1-(3-Cyano-3,3-diphenylpropyl)-4-phenylisonipecotic acid
	Difenoxilic acid
	Difenoxylic acid
	Lyspafen
	McN-JR-15403-11
	1-(3-Cyano-3,3-diphenylpropyl)-4-phenyl-4-piperidinecarboxylic acid
Inchi:	InChI=1S/C28H28N2O2/c29-22-28(24-12-6-2-7-13-24,25-14-8-3-9-15-25)18-21-30-19-16
InchiKey:	UFIVBRCCIRTJTN-UHFFFAOYSA-N
Formula:	C28H28N2O2
SMILES:	N#CC(CCN1CCC(C(=O)O)(c2ccccc2)CC1)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	424.54

Physical Properties

Property code	Value	Unit	Source
logp	5.005		Crippen Method
mcvol	342.040	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28782425&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume