

# Difenoxin

**Other names:**

Isonipectic 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-phenylisonipectic acid  
Difenoxilic acid  
Difenoxylic acid  
Lyspafen  
McN-JR-15403-11

**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]:** 424.53**CAS:** 28782-42-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.73		Crippen Method
logp	5.005		Crippen Method
mcvol	342.040	ml/mol	McGowan Method

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C28782425&Units=SI>**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

# Legend

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

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