

# DIFENOXIN

|                      |                                                                                                                                                                                                                                                                                                                                                                                               |
|----------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | Isonipectic acid, 1-(3-cyano-3,3-diphenylpropyl)-4-phenyl-<br>Diphenoxin<br>Difenoxine<br>Diphenoxylic acid<br>4-Piperidinecarboxylic acid, 1-(3-cyano-3,3-diphenylpropyl)-4-phenyl-<br>1-(3-Cyano-3,3-diphenylpropyl)-4-phenylisonipectic acid<br>Difenoxilic acid<br>Difenoxylic acid<br>Lyspafen<br>McN-JR-15403-11<br>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:           | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| Cheméo Relay (1.0):       |                                                                                                                                               |
| Cheméo Relay (1.0, beta): |                                                                                                                                               |
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C28782425&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C28782425&amp;Units=SI</a> |
| McGowan Method:           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| Crippen Method:           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                     |

# Legend

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

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