

Proheptazine

Other names: 1H-Azepin-4-ol, hexahydro-1,3-dimethyl-4-phenyl-, propanoate (ester)
1H-Azepin-4-ol, hexahydro-1,3-dimethyl-4-phenyl-, propionate (ester)
1H-Azepin-4-ol, hexahydro-1,3-dimethyl-4-phenyl-, propanoate
1,3-Dimethyl-4-phenyl-4-propionyloxyazacycloheptane
Dimepheprimine
WY-757

Inchi: InChI=1S/C17H25NO2/c1-4-16(19)20-17(15-9-6-5-7-10-15)11-8-12-18(3)13-14(17)2/h5-

InchiKey: ZXWAUWBYASJEOE-UHFFFAOYSA-N

Formula: C17H25NO2

SMILES: CCC(=O)OC1(c2ccccc2)CCCN(C)CC1C

Mol. weight [g/mol]: 275.39

CAS: 77-14-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.30		Crippen Method
logp	3.197		Crippen Method
mcvol	233.190	ml/mol	McGowan Method
rinpol	1920.00		NIST Webbook
rinpol	1937.00		NIST Webbook
rinpol	1920.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: 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=C77145&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcpol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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