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/ci990307l
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
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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