Allylprodine

Other names:	4-Piperidinol, 1-methyl-4-phenyl-3-(2-propenyl)-, propanoate (ester) 4-Piperidinol, 3-allyl-1-methyl-4-phenyl-, propionate (ester) Alperidine NIH 7440 Ro 2-7113 3-Allyl-1-methyl-4-phenyl-4-propionyloxypiperidine 1-Methyl-4-phenyl-3-(2-propenyl)-4-piperidinol propanoate Propionic acid, 3-allyl-1-methyl-4-phenyl-4-piperidyl ester «alpha»-3-Allyl-1-methyl-4-phenyl-4-propionoxypiperidine
Inchi:	InChI=1S/C18H25NO2/c1-4-9-16-14-19(3)13-12-18(16,21-17(20)5-2)15-10-7-6-8-11-15/h
InchiKey:	KGYFOSCXVAXULR-UHFFFAOYSA-N
Formula:	C18H25NO2
SMILES:	C=CCC1CN(C)CCC1(OC(=O)CC)c1ccccc1
Mol. weight [g/mol]:	287.40
CAS:	25384-17-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	3.363		Crippen Method
mcvol	242.980	ml/mol	McGowan Method
rinpol	1929.00		NIST Webbook

Sources

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=C25384172&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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