

Anileridine

Other names:	4-Piperidinecarboxylic acid, 1-[2-(4-aminophenyl)ethyl]-4-phenyl-, ethyl ester Isonipecotic acid, 1-(p-aminophenethyl)-4-phenyl-, ethyl ester Adopol Alidine Apodol Ethyl 1-(p-aminophenethyl)-4-phenylisonipecotate Ethyl 1-(4-aminophenethyl)-4-phenylisonipecotate Leritin Leritine Nipecotan 1-[2-(4-Aminophenyl)ethyl]-4-phenyl-4-piperidinecarboxylic acid ethyl ester Apidol 1-(p-Aminophenethyl)-4-phenylpiperidine-4-carboxylic acid ethyl ester
Inchi:	InChI=1S/C22H28N2O2/c1-2-26-21(25)22(19-6-4-3-5-7-19)13-16-24(17-14-22)15-12-18
InchiKey:	LKYQLAWMNBFNJT-UHFFFAOYSA-N
Formula:	C22H28N2O2
SMILES:	CCOC(=O)C1(c2ccccc2)CCN(CCc2ccc(N)cc2)CC1
Mol. weight [g/mol]:	352.47
CAS:	144-14-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.87		Crippen Method
logp	3.408		Crippen Method
mcvol	289.860	ml/mol	McGowan Method
rinpol	2839.00		NIST Webbook
rinpol	2845.00		NIST Webbook
rinpol	2850.00		NIST Webbook
rinpol	2839.00		NIST Webbook
rinpol	2850.00		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=C144149&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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