

Isradipine

Other names:	3,5-Pyridinedicarboxylic acid, 4-(4-benzofurazanyl)-1,4-dihydro-2,6-dimethyl-, methyl 1-methylethyl ester, (.+/-)- Isopropyl methyl (.+/-)-4-(4-benzofurazanyl)-1,4-dihydro-2,6-dimethyl-3,5-pyridinedicarboxylate DynaCirc Isrodipine Clivoten Dynacrine Esradin Isopropyl methyl (.+/-)-4-(4-benzofurazanyl)-1,4-dihydro-2,6-dimethyl-3,5-pyridinedicarboxylate Lomir PN-200-110 Prescal Rebriden (.+/-)-Isradipine 3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1,4-dihydro-2,6-dimethyl-, methyl 1-methylethyl ester 3,5-Pyridinedicarboxylic acid, 4-(4-benzofurazanyl)-1,4-dihydro-2,6-dimethyl-, methyl 1-methylethyl ester DynaCirc DynaCirc CR Isradipin PN 200
Inchi:	InChI=1S/C19H21N3O5/c1-9(2)26-19(24)15-11(4)20-10(3)14(18(23)25-5)16(15)12-7-6-8
InchiKey:	HMJIYCCIYRONP-UHFFFAOYSA-N
Formula:	C19H21N3O5
SMILES:	<chem>COC(=O)C1=C(C)NC(C)=C(C(=O)OC(C)C)C1c1cccc2nonc12</chem>
Mol. weight [g/mol]:	371.39
CAS:	75695-93-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.53		Crippen Method
logp	2.582		Crippen Method
mcvol	270.880	ml/mol	McGowan Method
rinpol	2578.89		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75695931&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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