

Neocinchophen

Other names:

4-Quinolinecarboxylic acid, 6-methyl-2-phenyl-, ethyl ester
Cinchoninic acid, 6-methyl-2-phenyl-, ethyl ester
Ethyl 2-phenyl-6-methylcinchoninate
Ethyl 6-methyl-2-phenyl-4-quinolinecarboxylate
Ethyl 6-methyl-2-phenylcinchoninate
Neoatophan
Neocincophen
Neomagnephen
Neophan
Neoquinophan
Neu-Nylofanol
Novatophan
Novo-rheumatophin
Tolysin
6-Methyl-2-phenylquinoline-4-carboxylic acid, ethyl ester
6-Methylcinchophen, ethyl ester

Inchi:

InChI=1S/C19H17NO2/c1-3-22-19(21)16-12-18(14-7-5-4-6-8-14)20-17-10-9-13(2)11-15(

InchiKey:

BUDBHJPMAXMLD-UHFFFAOYSA-N

Formula:

C19H17NO2

SMILES:

CCOC(=O)c1cc(-c2ccccc2)nc2ccc(C)cc12

Mol. weight [g/mol]:

291.34

CAS:

485-34-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.78		Crippen Method
logp	4.387		Crippen Method
mcvol	229.010	ml/mol	McGowan Method
rinpole	2495.00		NIST Webbook
rinpole	2495.00		NIST Webbook

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C485347&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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<https://www.chemeo.com/cid/99-678-1/Neocinchophen.pdf>

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