

Nimetazepam

Other names:

1,3-Dihydro-1-methyl-7-nitro-5-phenyl-2H-1,4-benzodiazepin-2-one
1-Methyl-5-phenyl-7-nitro-1,3-dihydro-2H-1,4-benzodiazepin-2-one
1-Methyl-7-nitro-5-phenyl-1,3-dihydro-2H-1,4-benzodiazepin-2-one
1-Methylnitrazepam
2H-1,4-Benzodiazepin-2-one, 1,3-dihydro-1-methyl-7-nitro-5-phenyl-
Elimin
Hypnon
Methylnitrazepam
Nitrazepam, methylated
Ro 5-3453
S 1530

Inchi:

InChI=1S/C16H13N3O3/c1-18-14-8-7-12(19(21)22)9-13(14)16(17-10-15(18)20)11-5-3-2

InchiKey:

GWUSZQUVEVMBPI-UHFFFAOYSA-N

Formula:

C16H13N3O3

SMILES:

CN1C(=O)CN=C(c2ccccc2)c2cc([N+](=O)[O-])ccc21

Mol. weight [g/mol]:

295.29

CAS:

2011-67-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Aqueous Solubility Prediction Method
log10ws	-3.80		Estimated Solubility Method
logp	2.409		Crippen Method
mcvol	212.570	ml/mol	McGowan Method
rinpol	2662.00		NIST Webbook
rinpol	2693.00		NIST Webbook
rinpol	2640.00		NIST Webbook
rinpol	2693.00		NIST Webbook
rinpol	2693.00		NIST Webbook
rinpol	2662.00		NIST Webbook
rinpol	2662.00		NIST Webbook
rinpol	2662.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2011678&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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