

Hyoscyamine

Other names:

(-)-Atropine
(S)-(-)-Hyoscyamine
(S)-Atropine
1-Hyoscyamine
1 «alpha»H,5«alpha»H-Tropan-3«alpha»-ol, (-)-tropate (ester)
1Â«alphaÂ»H,5Â«alphaÂ»H-Tropan-3Â«alphaÂ»-ol, (-)-tropate (ester)
Azabicyclo(3.2.1)oct-3-yl ester, (3(S)-endo)-
Benzeneacetic acid, «alpha»-(hydroxymethyl)-,
8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, [3(S)-endo]-
Benzeneacetic acid, A«alphaA»-(hydroxymethyl)-,
8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, [3(S)-endo]-
Cystospaz
Daturine
Duboisine
Hyocyamine
L-Hyoscamine
L-Hyoscyamine
L-Tropine tropate
Levsin
Levsinex SR
Tropic acid, (-)-, ester with tropine
Tropic acid, 1 «alpha»H,5«alpha»H-tropan-3«alpha»-yl ester, (-)-
Tropic acid, 1Â«alphaÂ»H,5Â«alphaÂ»H-tropan-3Â«alphaÂ»-yl ester, (-)-
Tropine, (-)-tropate
l-Atropine
l-Hyopscyamine

Inchi: InChI=1S/C17H23NO3/c1-18-13-7-8-14(18)10-15(9-13)21-17(20)16(11-19)12-5-3-2-4-6-
InchiKey: RKUNBYITZUJHSG-AUSYRVNMSA-N
Formula: C17H23NO3
SMILES: CN1C2CCC1CC(OC(=O)C(CO)c1cccc1)C2
Mol. weight [g/mol]: 289.37
CAS: 101-31-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.72		Aqueous Solubility Prediction Method
logp	1.931		Crippen Method
mvol	228.200	ml/mol	McGowan Method

rinpol	2174.00	NIST Webbook
rinpol	2146.00	NIST Webbook
rinpol	2205.00	NIST Webbook
rinpol	2168.00	NIST Webbook
rinpol	2170.00	NIST Webbook
rinpol	2146.00	NIST Webbook
rinpol	2174.00	NIST Webbook
rinpol	2170.00	NIST Webbook
rinpol	2210.00	NIST Webbook
rinpol	2170.00	NIST Webbook
rinpol	2168.00	NIST Webbook
rinpol	2192.00	NIST Webbook
rinpol	2170.00	NIST Webbook
rinpol	2174.00	NIST Webbook
rinpol	2125.00	NIST Webbook
rinpol	2174.00	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>

McGowan Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C101315&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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