Atropine

Other names:

(+,-)-Tropyl tropate
(.+/-.)-Atropine
(.+/-.)-Hyoscyamine
(.+/-.)-Tropyl tropate
(±)-Atropine
(±)-Hyoscyamine
(Â±)-Atropine
(Â±)-Hyoscyamine
1-«alpha»-H,5-«alpha»-H-Tropan-3-«alpha»-ol (.+/-.)-tropate
1-Â«alphaÂ»-H,5-Â«alphaÂ»-H-Tropan-3-Â«alphaÂ»-ol (.+/-.)-tropate
1«alpha»H,5«alpha»H-Tropan-3«alpha»-ol (.+/-.)-tropate (ester)
1«alpha»H,5«alpha»H-Tropan-3«alpha»-ol (±)-tropate
1Â«alphaÂ»H,5Â«alphaÂ»H-Tropan-3Â«alphaÂ»-ol (.+/-.)-tropate (ester)
1Â«alphaÂ»H,5Â«alphaÂ»H-Tropan-3Â«alphaÂ»-ol (Â±)-tropate
2-Phenylhydracrylic acid 3-«alpha»-tropanyl ester
2-Phenylhydracrylic acid 3-Â«alphaÂ»-tropanyl ester
8-Methyl-8-azabicyclo[3.2.1]oct-3-yl tropate
Atropin
Atropin-flexiolen
Atropina
Atropinol
Atropisol
Benzeneacetic acid, «alpha»-(hydroxymethyl)-, (3-endo)-8-methyl-8-azabicyclo(3.2.1)oct-3-yl ester
Benzeneacetic acid, «alpha»-(hydroxymethyl)-, 8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester endo-(.+/-.)-
Benzeneacetic acid, «alpha»-(hydroxymethyl)-, 8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester endo-(±)-
Benzeneacetic acid, A«alphaA»-(hydroxymethyl)-, (3-endo)-8-methyl-8-azabicyclo(3.2.1)oct-3-yl ester
Benzeneacetic acid, A«alphaA»-(hydroxymethyl)-, 8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester endo-(.+/-.)-
Benzeneacetic acid, A«alphaA»-(hydroxymethyl)-, 8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester endo-(Â±)-
DL-Hyoscyamine
DL-Tropanyl 2-hydroxy-1-phenylpropionate
DL-Tropyl tropate
Eyesules
Isopto-atropine
Tropic acid, 3-«alpha»-tropanyl ester
Tropic acid, 3-Â«alphaÂ»-tropanyl ester
Tropic acid, ester with tropine
Tropine tropate
«alpha»-(Hydroxymethyl)benzeneacetic acid 8-methyl-8-azabicyclo(3.2.1)oct-3-yl ester
«alpha»-(Hydroxymethyl)benzeneacetic acid 8-methyl-8-azabicyclo(3.2.1)oct-3-yl ester, endo-
«alpha»-(hydroxymethyl)-benzene acetic acid, (3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester (atropine)

«beta»-Phenyl-«gamma»-oxypropionsaeure-tropyl-ester

Â«alphaÂ»-(Hydroxymethyl)benzeneacetic acid 8-methyl-8-azabicyclo(3.2.1)oct-3-yl ester

Ã«alphaÃ»-(Hydroxymethyl)benzeneacetic acid 8-methyl-8-azabicyclo(3.2.1)oct-3-yl ester, endo-

Ã«alphaÃ»-(hydroxymethyl)-benzene acetic acid, (3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester (atropine)

Ã«betaÃ»-Phenyl-Ã«gammaÃ»-oxypropionsaeure-tropyl-ester

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-UHFFFAOYSA-N

Formula: C17H23NO3

SMILES: CN1C2CCC1CC(OC(=O)C(CO)c1ccccc1)C2

Mol. weight [g/mol]: 289.37

CAS: 51-55-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.00		Aqueous Solubility Prediction Method
logp	1.931		Crippen Method
mcvol	228.200	ml/mol	McGowan Method
rinpol	2175.00		NIST Webbook
rinpol	2184.00		NIST Webbook
rinpol	2145.00		NIST Webbook
rinpol	2183.00		NIST Webbook
rinpol	2169.00		NIST Webbook
rinpol	2147.00		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2169.00		NIST Webbook
rinpol	2199.00		NIST Webbook
rinpol	2194.00		NIST Webbook
rinpol	2169.00		NIST Webbook
rinpol	2202.00		NIST Webbook
rinpol	2202.00		NIST Webbook
rinpol	2169.00		NIST Webbook
rinpol	2175.00		NIST Webbook
rinpol	2147.00		NIST Webbook
rinpol	2145.00		NIST Webbook
rinpol	2199.00		NIST Webbook
rinpol	2199.00		NIST Webbook
rinpol	2169.00		NIST Webbook
rinpol	2147.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	35.50	kJ/mol	388.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C51558&Units=SI

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices