Haloperidol

Other names:

1-(3-p-Fluorobenzoylpropyl)-4-p-chlorophenyl-4-hydroxypiperidine
1-(4-Fluorophenyl)-4-[4-hydroxy-4-(4-chlorophenyl)-1-piperidinyl]-1-butanone (haloperidol)
1-Butanone, 4-[4-(4-chlorophenyl)-4-hydroxy-1-piperidinyl]-1-(4-fluorophenyl)-
4'-Fluoro-4-(4-(p-chlorophenyl)-4-hydroxypiperidinyl)butyrophenone
4'-Fluoro-4-(4-hydroxy-4-(4'-chlorophenyl)piperidino)butyrophenone
4-(4-(4-Chlorophenyl)-4-hydroxy-1-piperidinyl)-1-(4-fluorophenyl)-1-butanone
4-(4-(p-Chlorophenyl)-4-hydroxypiperidino)-4'-fluorobutyrophenone
4-(4-(para-Chlorophenyl)-4-hydroxypiperidino)-4'-fluorobutyrophenone
4-(4-Hydroxy-4'-chloro-4-phenylpiperidino)-4'-fluorobutyrophenone
ALDO
Aloperidin
Aloperidol
Aloperidolo
Aloperidon
Bioperidolo
Brotopon
Butyrophenone, 4'-fluoro-4-(4-(p-chlorophenyl)-4-hydroxypiperidino)-
Butyrophenone, 4-[4-(p-chlorophenyl)-4-hydroxypiperidino]-4'-fluoro-
Dozic
Einalon S
Eukystol
Galoperidol
Haldol
Halidol
Halojust
Halopal
Halopidol
Halopoidol
Halosten
Keselan
Lealgin compositum
Linton
McM-JR-1625
McN-JR-1625
Mixidol
Pekuces
Peluces
Pernox
R 1625
SC 170973

	Serenace
	Serenase
	Serenelfi
	Sernas
	Sernel
	Sigaperidol
	Ulcolind
	Uliolind
	Vesalium
	«gamma»-(4-(p-Chlorophenyl)-4-hydroxpiperidino)-p-fluorbutyrophenone
	Â«gammaÂ»-(4-(p-Chlorophenyl)-4-hydroxpiperidino)-p-fluorbutyrophenone
Inchi:	InChI=1S/C21H23ClFNO2/c22-18-7-5-17(6-8-18)21(26)11-14-24(15-12-21)13-1-2-20(25)
InchiKey:	LNEPOXFFQSENCJ-UHFFFAOYSA-N
Formula:	C21H23ClFNO2
SMILES:	O=C(CCCN1CCC(O)(c2ccc(Cl)cc2)CC1)c1ccc(F)cc1
Mol. weight [g/mol]:	375.86
CAS:	52-86-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.71		Aqueous Solubility Prediction Method
logp	4.426		Crippen Method
mcvol	279.800	ml/mol	McGowan Method
rinpol	2885.00		NIST Webbook
rinpol	3082.50		NIST Webbook
rinpol	2942.00		NIST Webbook
rinpol	2897.00		NIST Webbook
rinpol	2921.00		NIST Webbook
rinpol	2921.00		NIST Webbook
rinpol	2887.00		NIST Webbook
rinpol	2905.00		NIST Webbook
rinpol	2930.00		NIST Webbook
rinpol	2916.00		NIST Webbook
rinpol	2932.00		NIST Webbook
rinpol	2942.00		NIST Webbook
rinpol	2915.00		NIST Webbook
rinpol	2970.00		NIST Webbook
rinpol	2942.00		NIST Webbook
rinpol	2925.00		NIST Webbook

rinpol	2925.00		NIST Webbook
rinpol	2905.00		NIST Webbook
rinpol	2965.00		NIST Webbook
rinpol	2930.00		NIST Webbook
rinpol	2916.00		NIST Webbook
rinpol	2950.00		NIST Webbook
tf	423.02	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	48.00	kJ/mol	422.70	NIST Webbook

Sources

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=C52868&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tf: Normal melting (fusion) point