Moperone

Other names:	1-(4-fluorophenyl)-4-[4-hydroxy-4-(4-methylphenyl)piperidin-1-yl]butan-1-one
	1-Butanone, 1-(4-fluorophenyl)-4-[4-hydroxy-4-(4-methylphenyl)-1-piperidinyl]-
	4'-Fluoro-4-(4-hydroxy-4-p-tolylpiperidino)butyrophenone
	Butyrophenone, 4'-fluoro-4-(4-hydroxy-4-p-tolylpiperidino)-
	Luvatren
	Luvatrena
	Meperon
	Methylperidol
	Pregna-2,4-dien-20-yno[2,3-d]isoxazol-17-ol (danazol)
	R 1658
Inchi:	InChI=1S/C22H26FNO2/c1-17-4-8-19(9-5-17)22(26)12-15-24(16-13-22)14-2-3-21(25)18-
InchiKey:	AGAHNABIDCTLHW-UHFFFAOYSA-N
Formula:	C22H27NO2
SMILES:	Cc1ccc(C2(O)CCN(CCCC(=O)c3ccc(F)cc3)CC2)cc1
Mol. weight [g/mol]:	337.46
CAS:	1050-79-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.35		Aqueous Solubility Prediction Method
logp	4.081		Crippen Method
mcvol	281.650	ml/mol	McGowan Method
rinpol	2810.00		NIST Webbook
rinpol	2845.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	35.50	kJ/mol	501.80	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=C1050799&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