Bromperidol

Other names:	1-Butanone, 4-[4-(4-bromophenyl)-4-hydroxy-1-piperidinyl]-1-(4-fluorophenyl)- Butyrophenone, 4-(4-(p-bromophenyl)-4-hydroxypiperidino)-4'-fluoro- Bromoperidol 4-(4-(p-Bromophenyl)-4-hydroxypiperidino)-4'-fluorobutyrophenone 4-(4-(4-Bromophenyl)-4-hydroxypiperidino)-4'-fluorobutyrophenone 4-(4-(4-Bromophenyl)-4-hydroxy-1-piperidinyl)-1-(4-fluorophenyl)-1-butanone R 11333 1-Butanone, 4-[4-(4-bromophenyl)-4-hydroxy-1-piperidyl]-1-(4-fluorophenyl)- Azurene Impromen Tesoprel 1-(4-Fluorophenyl)-4-[4-hydroxy-4-(4-bromophenyl)-1-piperidinyl]-1-butanone (bromoperidol)
Inchi:	InChI=1S/C21H23BrFNO2/c22-18-7-5-17(6-8-18)21(26)11-14-24(15-12-21)13-1-2-20(25
InchiKey:	RKLNONIVDFXQRX-UHFFFAOYSA-N
Formula:	C21H23BrFNO2
SMILES:	O=C(CCCN1CCC(O)(c2ccc(Br)cc2)CC1)c1ccc(F)cc1
Mol. weight [g/mol]:	420.31
CAS:	10457-90-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.07		Crippen Method
logp	4.535		Crippen Method
mcvol	285.060	ml/mol	McGowan Method
rinpol	3023.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	50.80	kJ/mol	432.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10457906&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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