Pimozide

Other names:	2H-Benzimidazol-2-one, 1-[1-[4,4-bis(4-fluorophenyl)butyl]-4-piperidinyl]-1,3-dihydro- 2-Benzimidazolinone, 1-[1-[4,4-bis(p-fluorophenyl)butyl]-4-piperidyl]- R 6238 McN-JR 6238 Opiran Orap 1-(1-(4,4-Bis(p-fluorophenyl)butyl)-4-piperidyl)-2-benzimidazolinone 1-(4,4-Bis(p-fluorophenyl)butyl)-4-(2-oxo-1-benzimidazolinyl)piperidine 1-[1-[4,4-Bis(p-flurophenyl)butyl]-4-piperidyl]-2-benzimidazolinone NSC 170984 Primozide 1-[1-[4,4-bis(4-fluorophenyl)butyl]-4-piperidyl]-2-benzimidazolinone (pimozide)
Inchi:	InChI=1S/C28H29F2N3O/c29-22-11-7-20(8-12-22)25(21-9-13-23(30)14-10-21)4-3-17-32
InchiKey:	YVUQSNJEYSNKRX-UHFFFAOYSA-N
Formula:	C28H29F2N3O
SMILES:	O=c1[nH]c2ccccc2n1C1CCN(CCCC(c2ccc(F)cc2)c2ccc(F)cc2)CC1
Mol. weight [g/mol]:	461.55
CAS:	2062-78-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.50		Crippen Method
logp	5.375		Crippen Method
mcvol	347.430	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	46.90	kJ/mol	493.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2062784&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