Domperidone

Other names:	5-chloro-1-(1-(3-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)propyl)-4-piperidinyl)-1,3-dihydr
	5-chloro-1-(1-(3-(2-oxo-2,3-dihydro-1H-benzo[d]imidazol-1-yl)propyl)piperidin-4-yl)-1,3-di
Inchi:	InChI=1S/C22H24ClN5O2/c23-15-6-7-20-18(14-15)25-22(30)28(20)16-8-12-26(13-9-16)
InchiKey:	FGXWKSZFVQUSTL-UHFFFAOYSA-N
Formula:	C22H24ClN5O2
SMILES:	O=c1[nH]c2ccccc2n1CCCN1CCC(n2c(=O)[nH]c3cc(Cl)ccc32)CC1
Mol. weight [g/mol]:	425.92

Physical Properties

Property code	Value	Unit	Source
logp	2.389		Crippen Method
mcvol	306.020	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Domperidone Solubility in Aqueous Cosolvent Mixtures of N,N-Dimethylformamide, Isopropanol, Dimethyl Sulfoxide, and Ethanol: Thermodynamic Modeling and Preferential Solvation Analysis:	https://www.doi.org/10.1021/acs.jced.9b00216
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume