Midazolam

Other names:	Dormicum
	8-Chloro-6-(O-fluorophenyl)-1-methyl-4H-imidazo[1,5-a][1,4]-benzodiazepine
	4H-Imidazo[1,5-a][1,4]benzodiazepine, 8-chloro-6-(2-fluorophenyl)-1-methyl-
	8-Chloro-6-(2-fluorophenyl)-1-methyl-4H-imidazo[1,5-a][1,4]benzodiazepine
	59467-94-6 (maleate)
	59467-96-8 (hydrochloride)
Inchi:	InChI=1S/C18H13ClFN3/c1-11-21-9-13-10-22-18(14-4-2-3-5-16(14)20)15-8-12(19)6-7-17
InchiKey:	DDLIGBOFAVUZHB-UHFFFAOYSA-N
Formula:	C18H13ClFN3
SMILES:	Cc1ncc2n1-c1ccc(Cl)cc1C(c1ccccc1F)=NC2
Mol. weight [g/mol]:	325.77
CAS:	59467-70-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.52		Crippen Method
logp	4.324		Crippen Method
mcvol	226.290	ml/mol	McGowan Method
rinpol	2580.00		NIST Webbook
rinpol	2580.00		NIST Webbook
rinpol	2559.00		NIST Webbook
rinpol	2620.00		NIST Webbook
rinpol	2620.00		NIST Webbook
rinpol	2559.00		NIST Webbook
rinpol	2559.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59467708&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

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices