flubendazole

Other names:	methyl (5-(4-fluorobenzoyl)-1H-benzo[d]imidazol-2-yl)carbamate
Inchi:	InChI=1S/C16H12FN3O3/c1-23-16(22)20-15-18-12-7-4-10(8-13(12)19-15)14(21)9-2-5-1
InchiKey:	CPEUVMUXAHMANV-UHFFFAOYSA-N
Formula:	C16H12FN3O3
SMILES:	COC(=O)Nc1nc2ccc(C(=O)c3ccc(F)cc3)cc2[nH]1
Mol. weight [g/mol]:	313.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.96		Cheméo Relay (1.0)
logp	2.629		Crippen Method
mcvol	214.340	ml/mol	McGowan Method
tf	544.64	K	Cheméo Relay (1.0)

Sources

Solubility and preferential solvation of flubendazole dissolved in aqueous co-solvent mixtures of 1,4-dioxane, dimethyl sulfoxide, N,N-dimethylformamide and isopropanol:	https://www.doi.org/10.1016/j.jct.2019.04.001
Solubility Modeling and Solvent Effect for Flubendazole in 12 Neat Solvents:	https://www.doi.org/10.1021/acs.jced.8b01126
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point