Spiperone

Inchi: InChI=1S/C23H26FN3O2/c24-19-10-8-18(9-11-19)21(28)7-4-14-26-15-12-23(13-16-26)2
InchiKey: DKGZKTPJOSAWFA-UHFFFAOYSA-N
Formula: C23H26FN3O2
SMILES: O=C(CCCN1CCC2(CC1)C(=O)NCN2c1ccccc1)c1ccc(F)cc1
Mol. weight [g/mol]: 395.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.82		Cheméo Relay (1.0)
logp	3.217		Crippen Method
mcvol	300.540	ml/mol	McGowan Method
tf	431.64	K	Cheméo Relay (1.0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C749020&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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https://www.chemeo.com/cid/106-155-2/Spiperone.pdf