

MCPP, PFB

Inchi: InChI=1S/C17H14ClF5N2/c18-10-2-1-3-11(8-10)25-6-4-24(5-7-25)9-12-13(19)15(21)17(20)16
InchiKey: QIWCVOLBHFVJMQ-UHFFFAOYSA-N
Formula: C17H14ClF5N2
SMILES: Fc1c(F)c(F)c(CN2CCN(c3cccc(Cl)c3)CC2)c(F)c1F
Mol. weight [g/mol]: 376.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.55		Crippen Method
logp	4.358		Crippen Method
mcvol	233.060	ml/mol	McGowan Method
rinpol	1971.00		NIST Webbook
ripol	2752.00		NIST Webbook
ripol	2673.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R525867&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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