Fluazifop methyl ester

Inchi: InChI=1S/C16H14F3NO4/c1-10(15(21)22-2)23-12-4-6-13(7-5-12)24-14-8-3-11(9-20-14)1
InchiKey: IAUMNRCGDHLAMJ-UHFFFAOYSA-N
Formula: C16H14F3NO4
SMILES: COC(=O)C(C)Oc1ccc(Oc2ccc(C(F)(F)F)cn2)cc1
Mol. weight [g/mol]: 341.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.33		Crippen Method
logp	3.833		Crippen Method
mcvol	223.250	ml/mol	McGowan Method
rinpol	2030.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R72208&Units=SI

Legend

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