Warfarin, pentafluoropropionate

Inchi: InChI=1S/C22H15F5O5/c1-12(28)11-15(13-7-3-2-4-8-13)17-18(32-20(30)21(23,24)22(25
InchiKey: VDGXHNJCRNROJR-UHFFFAOYSA-N
Formula: C22H15F5O5
SMILES: CC(=O)CC(c1ccccc1)c1c(OC(=O)C(F)(F)C(F)(F)F)c2ccccc2oc1=O
Mol. weight [g/mol]: 454.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.74		Crippen Method
logp	5.007		Crippen Method
mcvol	283.460	ml/mol	McGowan Method
rinpol	2379.00		NIST Webbook
rinpol	2379.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375705&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.