2-Furoic acid, pentafluorophenyl ester

Inchi: InChI=1S/C11H3F5O3/c12-5-6(13)8(15)10(9(16)7(5)14)19-11(17)4-2-1-3-18-4/h1-3H
InchiKey: UIHCMTCYMQANRT-UHFFFAOYSA-N
Formula: C11H3F5O3
SMILES: O=C(Oc1c(F)c(F)c(F)c(F)c1F)c1ccco1
Mol. weight [g/mol]: 278.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.95		Crippen Method
logp	3.194		Crippen Method
mcvol	144.790	ml/mol	McGowan Method
rinpol	1385.00		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=U355170&Units=SI
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
rinpol: Non-polar retention indices