2-Furoic acid, anhydride with heptafluorobutyric acid

Inchi: InChI=1S/C9H3F7O4/c10-7(11,8(12,13)9(14,15)16)6(18)20-5(17)4-2-1-3-19-4/h1-3H
InchiKey: WWYBCVJFGVJROT-UHFFFAOYSA-N
Formula: C9H3F7O4
SMILES: O=C(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1ccco1
Mol. weight [g/mol]: 308.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.77		Crippen Method
logp	2.796		Crippen Method
mcvol	145.480	ml/mol	McGowan Method
rinpol	1018.00		NIST Webbook
rinpol	1018.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374902&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

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