3-Furoic acid, anhydride with trifluoroacetic acid

Inchi: InChI=1S/C7H3F3O4/c8-7(9,10)6(12)14-5(11)4-1-2-13-3-4/h1-3H
InchiKey: MSWXYWXXOSFSRF-UHFFFAOYSA-N
Formula: C7H3F3O4
SMILES: O=C(OC(=O)C(F)(F)F)c1ccoc1
Mol. weight [g/mol]: 208.09

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.30		Crippen Method
logp	1.525		Crippen Method
mcvol	110.220	ml/mol	McGowan Method
rinpol	891.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374896&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