2,3,4-Trifluorobenzoic acid, morpholide

Inchi: InChI=1S/C11H10F3NO2/c12-8-2-1-7(9(13)10(8)14)11(16)15-3-5-17-6-4-15/h1-2H,3-6H2
InchiKey: OYQXKOYUFQGWLM-UHFFFAOYSA-N
Formula: C11H10F3NO2
SMILES: O=C(c1ccc(F)c(F)c1F)N1CCOCC1
Mol. weight [g/mol]: 245.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.43		Crippen Method
logp	1.576		Crippen Method
mcvol	153.960	ml/mol	McGowan Method
rinpol	1588.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307172&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