3-Fluorobenzoic acid, morpholide

Inchi:	InChI=1S/C11H12FNO2/c12-10-3-1-2-9(8-10)11(14)13-4-6-15-7-5-13/h1-3,8H,4-7H2
InchiKey:	JZBARPSUMPODNT-UHFFFAOYSA-N
Formula:	C11H12FNO2
SMILES:	O=C(c1cccc(F)c1)N1CCOCC1
Mol. weight [g/mol]:	209.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.77		Crippen Method
logp	1.298		Crippen Method
mcvol	150.420	ml/mol	McGowan Method
rinpol	1626.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307161&Units=SI

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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