

2-Fluorobenzoic acid, morpholide

Inchi: InChI=1S/C11H12FNO2/c12-10-4-2-1-3-9(10)11(14)13-5-7-15-8-6-13/h1-4H,5-8H2
InchiKey: OIDNOKLCLGRXCW-UHFFFAOYSA-N
Formula: C11H12FNO2
SMILES: O=C(c1ccccc1F)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	1695.00		NIST Webbook
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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=U307077&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

Latest version available from:

<https://www.chemeo.com/cid/123-012-1/2-Fluorobenzoic-acid-morpholide.pdf>

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