

3-Trifluoromethylbenzoic acid, morpholide

Inchi: InChI=1S/C12H12F3NO2/c13-12(14,15)10-3-1-2-9(8-10)11(17)16-4-6-18-7-5-16/h1-3,8H
InchiKey: YWQNAFUPXWKYRS-UHFFFAOYSA-N
Formula: C12H12F3NO2
SMILES: O=C(c1cccc(C(F)(F)F)c1)N1CCOCC1
Mol. weight [g/mol]: 259.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Crippen Method
logp	2.178		Crippen Method
mcvol	168.050	ml/mol	McGowan Method
rinpol	1609.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U306932&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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<https://www.chemeo.com/cid/55-654-5/3-Trifluoromethylbenzoic-acid-morpholide.pdf>

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