1-Morpholinopropan-2-ol trifluoroacetate

Other names: 4-Morpholineethanol, «alpha»-methyl-, trifluoroacetate
4-(2-Trifluoroacetoxypropyl)morpholine
N-(2-Trifluoroacetoxypropyl)morpholine
Inchi: InChI=1S/C9H14F3NO3/c1-7(16-8(14)9(10,11)12)6-13-2-4-15-5-3-13/h7H,2-6H2,1H3
InchiKey: CGGIXRRSXIKIOT-UHFFFAOYSA-N
Formula: C9H14F3NO3
SMILES: CC(CN1CCOCC1)OC(=O)C(F)(F)F
Mol. weight [g/mol]: 241.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.78		Crippen Method
logp	0.813		Crippen Method
mcvol	155.410	ml/mol	McGowan Method
rinpol	1125.00		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=U373152&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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