hydroxyproline, trifluoroacetyl-isopropyl ester

Other names: Hydroxyproline, N-trifluoroacetyl, 1-methylethyl ester
Inchi: InChI=1S/C10H14F3NO4/c1-5(2)18-8(16)7-3-6(15)4-14(7)9(17)10(11,12)13/h5-7,15H,3-
InchiKey: OGJAAWUKJRYTCF-UHFFFAOYSA-N
Formula: C10H14F3NO4
SMILES: CC(C)OC(=O)C1CC(O)CN1C(=O)C(F)(F)F
Mol. weight [g/mol]: 269.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.37		Crippen Method
logp	0.462		Crippen Method
mcvol	171.070	ml/mol	McGowan Method
rinpol	1332.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1332.00		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=R84427&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