

proline, trifluoroacetyl-isopropyl ester

Other names: Proline, N-trifluoroacetyl, 1-methylethyl ester
Inchi: InChI=1S/C10H14F3NO3/c1-6(2)17-8(15)7-4-3-5-14(7)9(16)10(11,12)13/h6-7H,3-5H2,1-
InchiKey: AYEKUPVTUSWPOX-UHFFFAOYSA-N
Formula: C10H14F3NO3
SMILES: CC(C)OC(=O)C1CCCN1C(=O)C(F)(F)F
Mol. weight [g/mol]: 253.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.00		Crippen Method
logp	1.491		Crippen Method
mcvol	165.200	ml/mol	McGowan Method
rinpol	1283.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1331.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R84495&Units=SI>
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>

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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