

L-Proline, N-trifluoroacetyl-, 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C10H9F8NO3/c11-8(12,10(16,17)18)4-22-6(20)5-2-1-3-19(5)7(21)9(13,14)15/H
InchiKey: WUMSDKKXNIAXOC-UHFFFAOYSA-N
Formula: C10H9F8NO3
SMILES: O=C(OCC(F)(F)C(F)(F)F)C1CCCN1C(=O)C(F)(F)F
Mol. weight [g/mol]: 343.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.86		Crippen Method
logp	2.280		Crippen Method
mcvol	174.050	ml/mol	McGowan Method
rinpol	1187.60		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U352346&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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