

# L-Proline, 1-(trifluoroacetyl)-, butyl ester

<b>Other names:</b>	Proline, 1-(trifluoroacetyl)-, butyl ester, L-Pro, butyl ester, TFA Pro TFA Bu
<b>Inchi:</b>	InChI=1S/C11H16F3NO3/c1-2-3-7-18-9(16)8-5-4-6-15(8)10(17)11(12,13)14/h8H,2-7H2,
<b>InchiKey:</b>	BSVKMGHOOYHLQO-MRVPVSSYSA-N
<b>Formula:</b>	C11H16F3NO3
<b>SMILES:</b>	CCCCOC(=O)C1CCCN1C(=O)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	267.24
<b>CAS:</b>	2563-29-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.30		Crippen Method
logp	1.883		Crippen Method
mcvol	179.290	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2563293&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2563293&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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