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

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

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=C2563293&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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