

# Pro-hydroxy-Pro, butyl ester, TFA

**Inchi:** InChI=1S/C18H22F6N2O6/c1-2-3-9-31-14(28)11-5-4-8-25(11)13(27)10-6-7-12(32-16(30)  
**InchiKey:** ITDKFROWSJMGEZ-UHFFFAOYSA-N  
**Formula:** C18H22F6N2O6  
**SMILES:** CCCCOC(=O)C1CCCN1C(=O)C1CCC(OC(=O)C(F)(F)F)N1C(=O)C(F)(F)F  
**Mol. weight [g/mol]:** 476.37

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.72		Crippen Method
logp	2.306		Crippen Method
mcvol	291.360	ml/mol	McGowan Method
rinpola	2058.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R32058&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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  
**rinpola:** Non-polar retention indices

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