

# I-Proline, n-pentafluoropropionyl-, nonyl ester

**Inchi:** InChI=1S/C17H26F5NO3/c1-2-3-4-5-6-7-8-12-26-14(24)13-10-9-11-23(13)15(25)16(18,19)27-28-29-30-31  
**InchiKey:** IVTPIDXTLZRVPK-UHFFFAOYSA-N  
**Formula:** C17H26F5NO3  
**SMILES:** CCCCCCCCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)F  
**Mol. weight [g/mol]:** 387.39

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.13		Crippen Method
logp	4.469		Crippen Method
mcvol	267.370	ml/mol	McGowan Method
rinpol	1970.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=U321070&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  
**rinpol:** Non-polar retention indices

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