

# I-Proline, n-heptafluorobutyryl-, isohexyl ester

**Inchi:** InChI=1S/C15H20F7NO3/c1-9(2)5-4-8-26-11(24)10-6-3-7-23(10)12(25)13(16,17)14(18,19)20  
**InchiKey:** IHQXSPLYNGYVCE-UHFFFAOYSA-N  
**Formula:** C15H20F7NO3  
**SMILES:** CC(C)CCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)C(F)(F)F  
**Mol. weight [g/mol]:** 395.31

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -4.36   |        | Crippen Method |
| logp          | 3.790   |        | Crippen Method |
| mcvol         | 242.730 | ml/mol | McGowan Method |
| rinpol        | 1639.00 |        | NIST Webbook   |

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321101&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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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