l-Proline, n-pentafluoropropionyl-, heptadecyl ester

Inchi: InChI=1S/C25H42F5NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-34-22(32)21-18-1

InchiKey: OZWXRJTVTNJQOS-UHFFFAOYSA-N

Formula: C25H42F5NO3

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 499.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.48		Crippen Method
logp	7.590		Crippen Method
mcvol	380.090	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=U321077&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume