l-Proline, n-pentafluoropropionyl-, decyl ester

Inchi: InChI=1S/C18H28F5NO3/c1-2-3-4-5-6-7-8-9-13-27-15(25)14-11-10-12-24(14)16(26)17(1
InchiKey: VFMZYZJBMXRPJX-UHFFFAOYSA-N
Formula: C18H28F5NO3
SMILES: CCCCCCCCCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 401.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.55		Crippen Method
logp	4.859		Crippen Method
mcvol	281.460	ml/mol	McGowan Method
rinpol	2067.00		NIST Webbook

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=U321071&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices