L-Proline, N-(pentafluorobenzoyl)-, undecyl ester

Inchi: InChI=1S/C23H30F5NO3/c1-2-3-4-5-6-7-8-9-10-14-32-23(31)15-12-11-13-29(15)22(30)1
InchiKey: QNDKTRHRZMPDRZ-UHFFFAOYSA-N
Formula: C23H30F5NO3
SMILES: CCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 463.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.00		Crippen Method
logp	6.061		Crippen Method
mcvol	328.150	ml/mol	McGowan Method
rinpol	2694.00		NIST Webbook
rinpol	2694.00		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=U346301&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.