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

Inchi: InChI=1S/C29H42F5NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-38-29(37)21-18-1

InchiKey: QRBOVKBZVDQWBT-UHFFFAOYSA-N

Formula: C29H42F5NO3

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 547.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.51		Crippen Method
logp	8.401		Crippen Method
mcvol	412.690	ml/mol	McGowan Method
rinpol	3347.00		NIST Webbook
rinpol	3347.00		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=U346306&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.