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

Inchi: InChI=1S/C19H22F5NO3/c1-2-3-4-5-6-10-28-19(27)11-8-7-9-25(11)18(26)12-13(20)15(2

InchiKey: XKXZQUYCDOASGJ-UHFFFAOYSA-N

Formula: C19H22F5NO3

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

Mol. weight [g/mol]: 407.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.33		Crippen Method
logp	4.500		Crippen Method
mcvol	271.790	ml/mol	McGowan Method
rinpol	2285.00		NIST Webbook
rinpol	2285.00		NIST Webbook

Sources

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=U346297&Units=SI

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

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.