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

Inchi: InChI=1S/C14H12F5NO3/c1-2-23-14(22)6-4-3-5-20(6)13(21)7-8(15)10(17)12(19)11(18)9
InchiKey: GNHWBQBOWUKDON-UHFFFAOYSA-N
Formula: C14H12F5NO3
SMILES: CCOC(=O)C1CCCN1C(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 337.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.24		Crippen Method
logp	2.550		Crippen Method
mcvol	201.340	ml/mol	McGowan Method
rinpol	1820.00		NIST Webbook
rinpol	1820.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346290&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.