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

Inchi: InChI=1S/C17H18F5NO3/c1-2-3-4-8-26-17(25)9-6-5-7-23(9)16(24)10-11(18)13(20)15(22
InchiKey: GEZAMLBYTUNVNU-UHFFFAOYSA-N
Formula: C17H18F5NO3
SMILES: CCCCCOC(=O)C1CCCN1C(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 379.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.49		Crippen Method
logp	3.720		Crippen Method
mcvol	243.610	ml/mol	McGowan Method
rinpol	2092.00		NIST Webbook
rinpol	2092.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346294&Units=SI
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

Legend

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

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