

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

Inchi: InChI=1S/C16H16F5NO3/c1-2-3-7-25-16(24)8-5-4-6-22(8)15(23)9-10(17)12(19)14(21)13
InchiKey: GAGCKAJPRAJFTL-UHFFFAOYSA-N
Formula: C16H16F5NO3
SMILES: CCCCO(=O)C1CCCN1C(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 365.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.07		Crippen Method
logp	3.330		Crippen Method
mcvol	229.520	ml/mol	McGowan Method
rinpol	2005.00		NIST Webbook
rinpol	2005.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U346293&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

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