l-Proline, n-pentafluoropropionyl-, butyl ester

Inchi: InChI=1S/C12H16F5NO3/c1-2-3-7-21-9(19)8-5-4-6-18(8)10(20)11(13,14)12(15,16)17/h8
InchiKey: XJVGZAYTDSSEDR-UHFFFAOYSA-N
Formula: C12H16F5NO3
SMILES: CCCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 317.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.04		Crippen Method
logp	2.518		Crippen Method
mcvol	196.920	ml/mol	McGowan Method
rinpol	1490.00		NIST Webbook
rinpol	1490.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321064&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.