l-Proline, n-pentafluoropropionyl-, dodecyl ester

Inchi: InChI=1S/C20H32F5NO3/c1-2-3-4-5-6-7-8-9-10-11-15-29-17(27)16-13-12-14-26(16)18(2

InchiKey: IWBPBGFESXPXFQ-UHFFFAOYSA-N

Formula: C20H32F5NO3

SMILES: CCCCCCCCCCCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 429.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.39		Crippen Method
logp	5.639		Crippen Method
mcvol	309.640	ml/mol	McGowan Method
rinpol	2262.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321073&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