l-Proline, n-pentafluoropropionyl-, tetradecyl ester

Inchi: InChI=1S/C22H36F5NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-31-19(29)18-15-14-16-28(1

InchiKey: BCKPMVAXDWSJNB-UHFFFAOYSA-N

Formula: C22H36F5NO3

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

Mol. weight [g/mol]: 457.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.22		Crippen Method
logp	6.419		Crippen Method
mcvol	337.820	ml/mol	McGowan Method

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=U321074&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume