l-Proline, n-heptafluorobutyryl-, undecyl ester

Inchi: InChI=1S/C20H30F7NO3/c1-2-3-4-5-6-7-8-9-10-14-31-16(29)15-12-11-13-28(15)17(30)1
InchiKey: OQVONGCRLTXOFY-UHFFFAOYSA-N
Formula: C20H30F7NO3
SMILES: CCCCCCCCCCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 465.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.70		Crippen Method
logp	5.884		Crippen Method
mcvol	313.180	ml/mol	McGowan Method
rinpol	2163.00		NIST Webbook

Sources

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=U321105&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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