

I-Proline, n-heptafluorobutyryl-, dodecyl ester

Inchi: InChI=1S/C21H32F7NO3/c1-2-3-4-5-6-7-8-9-10-11-15-32-17(30)16-13-12-14-29(16)18(30)
InchiKey: JUZFIPAGYOTTJT-UHFFFAOYSA-N
Formula: C₂₁H₃₂F₇NO₃
SMILES: CCCCCCCCCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 479.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.12		Crippen Method
logp	6.274		Crippen Method
mcvol	327.270	ml/mol	McGowan Method
rinpol	2262.00		NIST Webbook
rinpol	2262.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321106&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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