l-Proline, n-heptafluorobutyryl-, heptyl ester

Inchi: InChI=1S/C16H22F7NO3/c1-2-3-4-5-6-10-27-12(25)11-8-7-9-24(11)13(26)14(17,18)15(1
InchiKey: WLNLBZHPZDPOMB-UHFFFAOYSA-N
Formula: C16H22F7NO3
SMILES: CCCCCCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 409.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.02		Crippen Method
logp	4.324		Crippen Method
mcvol	256.820	ml/mol	McGowan Method
rinpol	1779.00		NIST Webbook
rinpol	1779.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321102&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.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

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