l-Proline, n-heptafluorobutyryl-, propyl ester

Inchi: InChI=1S/C12H14F7NO3/c1-2-6-23-8(21)7-4-3-5-20(7)9(22)10(13,14)11(15,16)12(17,18
InchiKey: GRNGDZUDZHGQAW-UHFFFAOYSA-N
Formula: C12H14F7NO3
SMILES: CCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 353.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.35		Crippen Method
logp	2.763		Crippen Method
mcvol	200.460	ml/mol	McGowan Method
rinpol	1418.00		NIST Webbook
rinpol	1418.00		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=U321097&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

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