l-Proline, n-pentafluoropropionyl-, heptyl ester

Inchi: InChI=1S/C15H22F5NO3/c1-2-3-4-5-6-10-24-12(22)11-8-7-9-21(11)13(23)14(16,17)15(1
InchiKey: ROJQZZXMWSJHPZ-UHFFFAOYSA-N
Formula: C15H22F5NO3
SMILES: CCCCCCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 359.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.29		Crippen Method
logp	3.689		Crippen Method
mcvol	239.190	ml/mol	McGowan Method
rinpol	1758.00		NIST Webbook
rinpol	1758.00		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=U321068&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

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