l-Proline, n-heptafluorobutyryl-, butyl ester

Inchi: InChI=1S/C13H16F7NO3/c1-2-3-7-24-9(22)8-5-4-6-21(8)10(23)11(14,15)12(16,17)13(18
InchiKey: BNFVCWZVOYWCDS-UHFFFAOYSA-N
Formula: C13H16F7NO3
SMILES: CCCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 367.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.77		Crippen Method
logp	3.154		Crippen Method
mcvol	214.550	ml/mol	McGowan Method
rinpol	1508.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321099&Units=SI
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

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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