

I-Proline, n-pentafluoropropionyl-, octyl ester

Inchi: InChI=1S/C16H24F5NO3/c1-2-3-4-5-6-7-11-25-13(23)12-9-8-10-22(12)14(24)15(17,18)16
InchiKey: IQETVZHKHOYRJR-UHFFFAOYSA-N
Formula: C16H24F5NO3
SMILES: CCCCCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 373.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.71		Crippen Method
logp	4.079		Crippen Method
mcvol	253.280	ml/mol	McGowan Method
rinpol	1865.00		NIST Webbook
rinpol	1865.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321069&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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