

I-Proline, n-pentafluoropropionyl-, heptadecyl ester

Inchi: InChI=1S/C25H42F5NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-34-22(32)21-18-19
InchiKey: OZWXRJTVTNJQOS-UHFFFAOYSA-N
Formula: C25H42F5NO3
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 499.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.48		Crippen Method
logp	7.590		Crippen Method
mcvol	380.090	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U321077&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.cheméo.com/cid/72-294-6/I-Proline-n-pentafluoropropionyl-heptadecyl-ester.pdf>

Generated by Cheméo on 2024-04-20 15:34:59.600980023 +0000 UTC m=+15916548.521557337.

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