

I-Proline, n-heptafluorobutyryl-, octyl ester

Inchi: InChI=1S/C17H24F7NO3/c1-2-3-4-5-6-7-11-28-13(26)12-9-8-10-25(12)14(27)15(18,19)1
InchiKey: MQGCCDKQWWYMGS-UHFFFAOYSA-N
Formula: C17H24F7NO3
SMILES: CCCCCCCCOC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 423.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.44		Crippen Method
logp	4.714		Crippen Method
mcvol	270.910	ml/mol	McGowan Method
rinpol	1875.00		NIST Webbook
rinpol	1875.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321103&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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