

L-Proline, N-(3,4-difluorobenzoyl)-, tetradecyl ester

Inchi: InChI=1S/C26H39F2NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-19-32-26(31)24-15-14-18-29(2)
InchiKey: CSRFSBXLWMWTHQ-UHFFFAOYSA-N
Formula: C26H39F2NO3
SMILES: CCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 451.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.26		Crippen Method
logp	6.814		Crippen Method
mcvol	365.110	ml/mol	McGowan Method
rinsol	3214.00		NIST Webbook
rinsol	3214.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U345913&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinsol: Non-polar retention indices

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