

L-Proline, N-(2,4-difluorobenzoyl)-, octyl ester

Inchi: InChI=1S/C20H27F2NO3/c1-2-3-4-5-6-7-13-26-20(25)18-9-8-12-23(18)19(24)16-11-10-1
InchiKey: MDDQYQWFMKKVRK-UHFFFAOYSA-N
Formula: C20H27F2NO3
SMILES: CCCCCCOC(=O)C1CCCN1C(=O)c1ccc(F)cc1F
Mol. weight [g/mol]: 367.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.75		Crippen Method
logp	4.473		Crippen Method
mcvol	280.570	ml/mol	McGowan Method
rmpol	2529.00		NIST Webbook
rmpol	2529.00		NIST Webbook

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=U346039&Units=SI>

Legend

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

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