

Isonipecotic acid, N-(2,5-difluorobenzoyl)-, pentadecyl ester

Inchi: InChI=1S/C28H43F2NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-21-34-28(33)23-17-19-31(2)
InchiKey: IWLLGYKSRCASBZ-UHFFFAOYSA-N
Formula: C28H43F2NO3
SMILES: CCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2cc(F)ccc2F)CC1
Mol. weight [g/mol]: 479.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.75		Crippen Method
logp	7.451		Crippen Method
mcvol	393.290	ml/mol	McGowan Method
rinpol	3549.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361423&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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