

Isonipecotic acid, N-(2,4-difluorobenzoyl)-, tridecyl ester

Inchi: InChI=1S/C26H39F2NO3/c1-2-3-4-5-6-7-8-9-10-11-12-19-32-26(31)21-15-17-29(18-16-20)
InchiKey: KCOQAFNVUQSYTB-UHFFFAOYSA-N
Formula: C₂₆H₃₉F₂NO₃
SMILES: CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(F)cc2F)CC1
Mol. weight [g/mol]: 451.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.91		Crippen Method
logp	6.671		Crippen Method
mcvol	365.110	ml/mol	McGowan Method
rmpol	3300.00		NIST Webbook
rmpol	3300.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361376&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
rmpol: Non-polar retention indices

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