

# Isonipecotic acid, N-(3,4-difluorobenzoyl)-, tridecyl ester

<b>Inchi:</b>	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)
<b>InchiKey:</b>	KKRCLACOMBSFHM-UHFFFAOYSA-N
<b>Formula:</b>	C26H39F2NO3
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(F)c(F)c2)CC1
<b>Mol. weight [g/mol]:</b>	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
rinpola	3339.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U361275&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361275&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

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