

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

Inchi: InChI=1S/C27H41F2NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-20-33-27(32)22-16-18-30(19-1
InchiKey: VKBMCKCEZMIBHH-UHFFFAOYSA-N
Formula: C27H41F2NO3
SMILES: CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(F)cc2F)CC1
Mol. weight [g/mol]: 465.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.33		Crippen Method
logp	7.061		Crippen Method
mcvol	379.200	ml/mol	McGowan Method
rmpol	3402.00		NIST Webbook
rmpol	3402.00		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=U361377&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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