

Isonipecotic acid, N-(4-fluorobenzoyl)-, decyl ester

Inchi: InChI=1S/C23H34FNO3/c1-2-3-4-5-6-7-8-9-18-28-23(27)20-14-16-25(17-15-20)22(26)19
InchiKey: VHZJBVUWMLULNB-UHFFFAOYSA-N
Formula: C23H34FNO3
SMILES: CCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(F)cc2)CC1
Mol. weight [g/mol]: 391.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.32		Crippen Method
logp	5.362		Crippen Method
mcvol	321.070	ml/mol	McGowan Method
rinpol	3061.00		NIST Webbook
rinpol	3061.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361077&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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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