

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

Inchi: InChI=1S/C24H37NO3/c1-3-4-5-6-7-8-9-10-19-28-24(27)22-15-17-25(18-16-22)23(26)21
InchiKey: VOBQITLNZDHJAJ-UHFFFAOYSA-N
Formula: C24H37NO3
SMILES: CCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(C)cc2)CC1
Mol. weight [g/mol]: 387.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.47		Crippen Method
logp	5.531		Crippen Method
mcvol	333.390	ml/mol	McGowan Method
rinpole	3226.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361122&Units=SI>
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>

Legend

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

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