

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

Inchi: InChI=1S/C26H41NO3/c1-3-4-5-6-7-8-9-10-11-12-21-30-26(29)24-17-19-27(20-18-24)25
InchiKey: VOZNMJGQKOAYOP-UHFFFAOYSA-N
Formula: C26H41NO3
SMILES: CCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(C)cc2)CC1
Mol. weight [g/mol]: 415.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.30		Crippen Method
logp	6.311		Crippen Method
mcvol	361.570	ml/mol	McGowan Method
rinpol	3436.00		NIST Webbook
rinpol	3436.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361124&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
rinpol: Non-polar retention indices

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