

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

Inchi:	InChI=1S/C23H35NO3/c1-3-4-5-6-7-8-9-18-27-23(26)21-14-16-24(17-15-21)22(25)20-12
InchiKey:	CBZXISJHYPKWSZ-UHFFFAOYSA-N
Formula:	C23H35NO3
SMILES:	CCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(C)cc2)CC1
Mol. weight [g/mol]:	373.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.05		Crippen Method
logp	5.141		Crippen Method
mcvol	319.300	ml/mol	McGowan Method
rinpola	3121.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361121&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
rinpola:	Non-polar retention indices

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