

Isonipecotic acid, N-(3-methylbenzoyl)-, nonyl ester

Inchi:	InChI=1S/C23H35NO3/c1-3-4-5-6-7-8-9-17-27-23(26)20-13-15-24(16-14-20)22(25)21-12
InchiKey:	ACKZJKXCSYWUSH-UHFFFAOYSA-N
Formula:	C23H35NO3
SMILES:	CCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(C)c2)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
rinpol	3094.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361104&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/10-714-7/Isonipecotic-acid-N-3-methylbenzoyl-nonyl-ester.pdf>

Generated by Cheméo on 2025-12-24 08:22:56.373421289 +0000 UTC m=+6312773.903461943.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.