

Isonipecotic acid, N-(2-methoxybenzoyl)-, nonyl ester

Inchi:	InChI=1S/C23H35NO4/c1-3-4-5-6-7-8-11-18-28-23(26)19-14-16-24(17-15-19)22(25)20-1
InchiKey:	YGSPLNSMMLCYNZ-UHFFFAOYSA-N
Formula:	C23H35NO4
SMILES:	CCCCCCCCCOC(=O)C1CCN(C(=O)c2ccccc2OC)CC1
Mol. weight [g/mol]:	389.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.69		Crippen Method
logp	4.841		Crippen Method
mcvol	325.170	ml/mol	McGowan Method
rinpola	3132.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361193&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/36-959-8/Isonipecotic-acid-N-2-methoxybenzoyl-nonyl-ester.pdf>

Generated by Cheméo on 2024-04-27 09:12:12.855450115 +0000 UTC m=+16498381.776027435.

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