

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

Inchi: InChI=1S/C19H27NO4/c1-3-4-7-14-24-19(22)15-10-12-20(13-11-15)18(21)16-8-5-6-9-17
InchiKey: MHECOSDQLJKSFI-UHFFFAOYSA-N
Formula: C19H27NO4
SMILES: CCCCCOC(=O)C1CCN(C(=O)c2ccccc2OC)CC1
Mol. weight [g/mol]: 333.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.02		Crippen Method
logp	3.281		Crippen Method
mcvol	268.810	ml/mol	McGowan Method
rinpol	2696.00		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=U361188&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/53-405-3/Isonipecotic-acid-N-2-methoxybenzoyl-pentyl-ester.pdf>

Generated by Cheméo on 2025-12-24 09:07:38.40122783 +0000 UTC m=+6315455.931268483.

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