

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

Inchi: InChI=1S/C20H29NO3/c1-15(2)6-5-13-24-20(23)17-9-11-21(12-10-17)19(22)18-8-4-7-16
InchiKey: MNMOVQSFXROBNQ-UHFFFAOYSA-N
Formula: C20H29NO3
SMILES: Cc1cccc(C(=O)N2CCC(C(=O)OCCCC(C)C)CC2)c1
Mol. weight [g/mol]: 331.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.55		Crippen Method
logp	3.827		Crippen Method
mcvol	277.030	ml/mol	McGowan Method
rinpol	2715.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361100&Units=SI>
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>

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/66-175-5/Isonipecotic-acid-N-3-methylbenzoyl-isohexyl-ester.pdf>

Generated by Cheméo on 2025-12-24 12:13:37.396159882 +0000 UTC m=+6326614.926200551.

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