

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

Inchi: InChI=1S/C20H29NO4/c1-15(2)6-5-13-25-20(23)16-9-11-21(12-10-16)19(22)17-7-4-8-18
InchiKey: HOHSXULALIUSQO-UHFFFAOYSA-N
Formula: C20H29NO4
SMILES: COc1cccc(C(=O)N2CCC(C(=O)OCCCC(C)C)CC2)c1
Mol. weight [g/mol]: 347.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	3.527		Crippen Method
mcvol	282.900	ml/mol	McGowan Method
rinpol	2860.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361177&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

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