

Isonipectic acid, N-(3-methoxybenzoyl)-, nonyl ester

Inchi: InChI=1S/C23H35NO4/c1-3-4-5-6-7-8-9-17-28-23(26)19-13-15-24(16-14-19)22(25)20-11
InchiKey: OHXOKFBVSNVMOZ-UHFFFAOYSA-N
Formula: C23H35NO4
SMILES: CCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(OC)c2)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
rinpol	3232.00		NIST Webbook
rinpol	3232.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361181&Units=SI>
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>

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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