

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

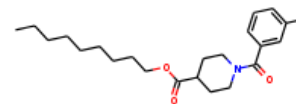
InChI: InChI=1S/C23H35NO3/c1-3-4-5-6-7-8-9-17-27-23(26)20-13-15-24(16-14-20)22(25)21-12-10-11-19(2)18-21/h10-12,18,20H,3-9,13-17H2,1-2H3

InChI Key: ACKZJKXCSYWUSH-UHFFFAOYSA-N

Formula: C23H35NO3

SMILES: CCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(C)c2)CC1

Molecular Weight: 373.53



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	5.14		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C23H35NO3/c1-3-4-5-6-7-8-9-17-27-23\(26\)20-13-15-24\(16-14-20\)22\(25\)21-12-10-11-19\(2\)18-21/h10-12,18,20H,3-9,13-17H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C23H35NO3/c1-3-4-5-6-7-8-9-17-27-23(26)20-13-15-24(16-14-20)22(25)21-12-10-11-19(2)18-21/h10-12,18,20H,3-9,13-17H2,1-2H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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