

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

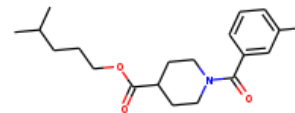
InChI: InChI=1S/C20H29NO3/c1-15(2)6-5-13-24-20(23)17-9-11-21(12-10-17)19(22)18-8-4-7-16(3)14-18/h4,7-8,14-15,17H,5-6,9-13H2,1-3H3

InChI Key: MNMOVQSFXROBNQ-UHFFFAOYSA-N

Formula: C20H29NO3

SMILES: Cc1cccc(C(=O)N2CCC(C(=O)OCCCC(C)C)CC2)c1

Molecular Weight: 331.45



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	3.83		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/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\(3\)14-18/h4,7-8,14-15,17H,5-6,9-13H2,1-3H3](http://webbook.nist.gov/cgi/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(3)14-18/h4,7-8,14-15,17H,5-6,9-13H2,1-3H3)

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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