

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

Inchi:	InChI=1S/C24H37NO3/c1-3-4-5-6-7-8-9-10-18-28-24(27)21-14-16-25(17-15-21)23(26)22
InchiKey:	TWUAQGNUMVCELKP-UHFFFAOYSA-N
Formula:	C24H37NO3
SMILES:	CCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(C)c2)CC1
Mol. weight [g/mol]:	387.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.47		Crippen Method
logp	5.531		Crippen Method
mcvol	333.390	ml/mol	McGowan Method
rinsol	3199.00		NIST Webbook
rinsol	3199.00		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=U361105&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinsol:	Non-polar retention indices

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