

Isonipectic acid, N-(2-methoxybenzoyl)-, decyl ester

Inchi: InChI=1S/C24H37NO4/c1-3-4-5-6-7-8-9-12-19-29-24(27)20-15-17-25(18-16-20)23(26)21
InchiKey: NSYZMNCZBSBGSN-UHFFFAOYSA-N
Formula: C24H37NO4
SMILES: CCCCCCCCCOC(=O)C1CCN(C(=O)c2ccccc2OC)CC1
Mol. weight [g/mol]: 403.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.11		Crippen Method
logp	5.231		Crippen Method
mcvol	339.260	ml/mol	McGowan Method
rinpola	3236.00		NIST Webbook
rinpola	3236.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361194&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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