

Isonipectic acid, N-(3-bromobenzoyl)-, undecyl ester

Inchi: InChI=1S/C24H36BrNO3/c1-2-3-4-5-6-7-8-9-10-18-29-24(28)20-14-16-26(17-15-20)23(2)
InchiKey: XKCDGCLFMQDRMH-UHFFFAOYSA-N
Formula: C24H36BrNO3
SMILES: CCCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(Br)c2)CC1
Mol. weight [g/mol]: 466.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.57		Crippen Method
logp	6.375		Crippen Method
mcvol	350.890	ml/mol	McGowan Method
rmpol	3511.00		NIST Webbook
rmpol	3511.00		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=U361519&Units=SI>

Legend

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

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