

Isonipectic acid, N-(2-chlorobenzoyl)-, dodecyl ester

Inchi: InChI=1S/C25H38ClNO3/c1-2-3-4-5-6-7-8-9-10-13-20-30-25(29)21-16-18-27(19-17-21)2
InchiKey: JWIJOPAEBWCDKF-UHFFFAOYSA-N
Formula: C25H38ClNO3
SMILES: CCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccccc2Cl)CC1
Mol. weight [g/mol]: 436.03

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.51		Crippen Method
logp	6.656		Crippen Method
mcvol	359.720	ml/mol	McGowan Method
rmpol	3471.00		NIST Webbook
rmpol	3471.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.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=U361167&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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