

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

Inchi:	InChI=1S/C21H30ClNO3/c1-2-3-4-5-6-9-16-26-21(25)17-12-14-23(15-13-17)20(24)18-10
InchiKey:	GZQWHCNEZNNRRL-UHFFFAOYSA-N
Formula:	C21H30ClNO3
SMILES:	CCCCCCCCOC(=O)C1CCN(C(=O)c2ccccc2Cl)CC1
Mol. weight [g/mol]:	379.92

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.84		Crippen Method
logp	5.096		Crippen Method
mcvol	303.360	ml/mol	McGowan Method
rinsol	3042.00		NIST Webbook
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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=U361163&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
rinsol:	Non-polar retention indices

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