

Isonipecotic acid, N-(2-chlorobenzoyl)-, heptyl ester

Inchi: InChI=1S/C20H28ClNO3/c1-2-3-4-5-8-15-25-20(24)16-11-13-22(14-12-16)19(23)17-9-6-
InchiKey: CARCIGJCMDMUCJ-UHFFFAOYSA-N
Formula: C20H28ClNO3
SMILES: CCCCCCOC(=O)C1CCN(C(=O)c2ccccc2Cl)CC1
Mol. weight [g/mol]: 365.89

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.42		Crippen Method
logp	4.706		Crippen Method
mcvol	289.270	ml/mol	McGowan Method
rinpol	2936.00		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=U361162&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
rinpol: Non-polar retention indices

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