

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

Inchi: InChI=1S/C19H26ClNO3/c1-14(2)6-5-13-24-19(23)15-9-11-21(12-10-15)18(22)16-7-3-4-
InchiKey: PZJIBEYUVZLSPA-UHFFFAOYSA-N
Formula: C19H26ClNO3
SMILES: CC(C)CCCOC(=O)C1CCN(C(=O)c2ccccc2Cl)CC1
Mol. weight [g/mol]: 351.87

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.76 | | Crippen Method |
| logp | 4.172 | | Crippen Method |
| mcvol | 275.180 | ml/mol | McGowan Method |
| rinpol | 2767.00 | | NIST Webbook |
| rinpol | 2767.00 | | 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=U361160&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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