

# Isonipecotic acid, N-(5-chlorovaleryl)-, isohexyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C17H30ClNO3/c1-14(2)6-5-13-22-17(21)15-8-11-19(12-9-15)16(20)7-3-4-10-1 |
| <b>InchiKey:</b>            | OTQJYMXMTBSYQF-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C17H30ClNO3  |
| <b>SMILES:</b>              | CC(C)CCCOC(=O)C1CCN(C(=O)CCCCCl)CC1  |
| <b>Mol. weight [g/mol]:</b> | 331.88   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -3.71   |        | Crippen Method |
| logp          | 3.613   |        | Crippen Method |
| mcvol         | 270.760 | ml/mol | McGowan Method |
| rinpola       | 2617.00 |        | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U361007&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361007&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/26-314-4/Isonipecotic-acid-N-5-chlorovaleryl-isohexyl-ester.pdf>

Generated by Cheméo on 2024-04-25 06:12:36.23334066 +0000 UTC m=+16314805.153917972.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.