

# 1-(3-chlorophenyl)piperazine, acetyl

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | mCPP, AC<br>Nefazodone-M (N-desalkyl-) AC  |
| <b>Inchi:</b>               | InChI=1S/C12H15ClN2O/c1-10(16)14-5-7-15(8-6-14)12-4-2-3-11(13)9-12/h2-4,9H,5-8H2 |
| <b>InchiKey:</b>            | FGZISPCFLHSBOQ-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C12H15ClN2O  |
| <b>SMILES:</b>              | CC(=O)N1CCN(c2cccc(Cl)c2)CC1   |
| <b>Mol. weight [g/mol]:</b> | 238.71   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -1.98   |        | Crippen Method |
| logp          | 2.008   |        | Crippen Method |
| mcvol         | 179.090 | ml/mol | McGowan Method |
| rinpol        | 2265.00 |        | NIST Webbook   |
| rinpol        | 2265.00 |        | NIST Webbook   |
| rinpol        | 2265.00 |        | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <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=U379022&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U379022&amp;Units=SI</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>rinpol:</b>  | Non-polar retention indices         |

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