

# 4-M-chloroanilino-6-methyl-1,3,3a,7-tetrazaindene

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C12H10ClN5/c1-8-5-11(18-12(16-8)14-7-15-18)17-10-4-2-3-9(13)6-10/h2-7,17 |
| <b>InchiKey:</b>            | JAHTUKQLGZAZIX-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C12H10ClN5  |
| <b>SMILES:</b>              | Cc1cc(Nc2cccc(Cl)c2)n2ncnc2n1   |
| <b>Mol. weight [g/mol]:</b> | 259.69  |
| <b>CAS:</b>                 | 104997-66-2   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -4.70   |        | Crippen Method |
| logp          | 2.830   |        | Crippen Method |
| mcvol         | 179.400 | ml/mol | McGowan Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C104997662&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C104997662&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>                               |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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     |

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