

# Methanone,(2-chlorophenyl)-2-pyridinyl-

|                      |                                                                     |
|----------------------|---------------------------------------------------------------------|
| Other names:         | 2-(2-Chlorobenzoyl)-pyridine                                        |
| Inchi:               | InChI=1S/C12H8ClNO/c13-10-6-2-1-5-9(10)12(15)11-7-3-4-8-14-11/h1-8H |
| InchiKey:            | XSPNJXJVXUZKPE-UHFFFAOYSA-N                                         |
| Formula:             | C12H8ClNO                                                           |
| SMILES:              | O=C(c1ccccc1)c1ccccc1Cl                                             |
| Mol. weight [g/mol]: | 217.65                                                              |
| CAS:                 | 1694-57-1                                                           |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| ie            | 8.98    | eV     | NIST Webbook   |
| log10ws       | -3.88   |        | Crippen Method |
| logp          | 2.966   |        | Crippen Method |
| mcvol         | 156.210 | ml/mol | McGowan Method |

## Sources

|                 |                                                                                                                                             |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1694571&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1694571&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                   |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |

## Legend

|          |                                     |
|----------|-------------------------------------|
| ie:      | Ionization energy                   |
| log10ws: | Log10 of Water solubility in mol/l  |
| logp:    | Octanol/Water partition coefficient |
| mcvol:   | McGowan's characteristic volume     |

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