

# Benzene, 4-chloro-1,2-dimethyl-

|                      |                                                                                                                                   |
|----------------------|-----------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 1-Chloro-3,4-dimethylbenzene<br>4-Chloro-1,2-dimethylbenzene<br>4-Chloro-o-xylene<br>4-Chloro-ortho-xylene<br>o-Xylene, 4-chloro- |
| Inchi:               | InChI=1S/C8H9Cl/c1-6-3-4-8(9)5-7(6)2/h3-5H,1-2H3                                                                                  |
| InchiKey:            | HNQLMBJUMVLFCF-UHFFFAOYSA-N                                                                                                       |
| Formula:             | C8H9Cl                                                                                                                            |
| SMILES:              | Cc1ccc(Cl)cc1C                                                                                                                    |
| Mol. weight [g/mol]: | 140.61                                                                                                                            |
| CAS:                 | 615-60-1                                                                                                                          |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 97.70   | kJ/mol  | Joback Method  |
| hf            | -10.60  | kJ/mol  | Joback Method  |
| hfus          | 13.94   | kJ/mol  | Joback Method  |
| hvap          | 41.39   | kJ/mol  | Joback Method  |
| log10ws       | -3.11   |         | Crippen Method |
| logp          | 2.957   |         | Crippen Method |
| mcvol         | 112.060 | ml/mol  | McGowan Method |
| pc            | 3372.36 | kPa     | Joback Method  |
| rinpol        | 1075.00 |         | NIST Webbook   |
| rinpol        | 1073.00 |         | NIST Webbook   |
| rinpol        | 1084.00 |         | NIST Webbook   |
| tb            | 495.20  | K       | NIST Webbook   |
| tc            | 676.11  | K       | Joback Method  |
| tf            | 261.30  | K       | Joback Method  |
| vc            | 0.424   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 202.65 | J/mol×K | 456.51          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 252.92    | J/mol×K | 639.51 | Joback Method |
| cpg   | 244.00    | J/mol×K | 602.91 | Joback Method |
| cpg   | 234.54    | J/mol×K | 566.31 | Joback Method |
| cpg   | 224.50    | J/mol×K | 529.71 | Joback Method |
| cpg   | 213.88    | J/mol×K | 493.11 | Joback Method |
| cpg   | 261.31    | J/mol×K | 676.11 | Joback Method |
| dvisc | 0.0002426 | Pa×s    | 456.51 | Joback Method |
| dvisc | 0.0002952 | Pa×s    | 423.98 | Joback Method |
| dvisc | 0.0003710 | Pa×s    | 391.44 | Joback Method |
| dvisc | 0.0004860 | Pa×s    | 358.90 | Joback Method |
| dvisc | 0.0006718 | Pa×s    | 326.37 | Joback Method |
| dvisc | 0.0009978 | Pa×s    | 293.84 | Joback Method |
| dvisc | 0.0016353 | Pa×s    | 261.30 | Joback Method |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.24147e+01                   |
| Coeff. B                    | -3.30710e+03                  |
| Coeff. C                    | -7.10180e+01                  |
| Temperature range (K), min. | 343.72                        |
| Temperature range (K), max. | 536.59                        |

## Sources

|                                      |                                                                                                                                                                                         |
|--------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Joback Method:                       | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                                                                   |
| McGowan Method:                      | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                                                                   |
| NIST Webbook:                        | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C615601&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C615601&amp;Units=SI</a>                                               |
| The Yaws Handbook of Vapor Pressure: | <a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a> |
| Crippen Method:                      | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                                                               |
| Crippen Method:                      | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                                                                       |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <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>pc:</b>      | Critical Pressure                               |
| <b>pvap:</b>    | Vapor pressure                                  |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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