

# Benzene, 1,3-dichloro-5-(chloromethyl)-

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C7H5Cl3/c8-4-5-1-6(9)3-7(10)2-5/h1-3H,4H2 |
| <b>InchiKey:</b>            | ZFLRKAMKGYNFPH-UHFFFAOYSA-N                        |
| <b>Formula:</b>             | C7H5Cl3  |
| <b>SMILES:</b>              | ClCc1cc(Cl)cc(Cl)c1                                |
| <b>Mol. weight [g/mol]:</b> | 195.47   |
| <b>CAS:</b>                 | 3290-06-0  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 65.42   | kJ/mol  | Joback Method  |
| hf            | -21.44  | kJ/mol  | Joback Method  |
| hfus          | 19.74   | kJ/mol  | Joback Method  |
| hvap          | 47.93   | kJ/mol  | Joback Method  |
| log10ws       | -3.87   |         | Crippen Method |
| logp          | 3.732   |         | Crippen Method |
| mcvol         | 122.450 | ml/mol  | McGowan Method |
| pc            | 3460.21 | kPa     | Joback Method  |
| tb            | 508.49  | K       | Joback Method  |
| tc            | 743.54  | K       | Joback Method  |
| tf            | 309.87  | K       | Joback Method  |
| vc            | 0.467   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 208.02    | J/molxK | 508.49          | Joback Method |
| cpg           | 216.67    | J/molxK | 547.67          | Joback Method |
| cpg           | 224.73    | J/molxK | 586.84          | Joback Method |
| cpg           | 232.23    | J/molxK | 626.02          | Joback Method |
| cpg           | 239.19    | J/molxK | 665.19          | Joback Method |
| cpg           | 245.65    | J/molxK | 704.37          | Joback Method |
| cpg           | 251.62    | J/molxK | 743.54          | Joback Method |
| dvisc         | 0.0017070 | Paxs    | 309.87          | Joback Method |
| dvisc         | 0.0010988 | Paxs    | 342.97          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0007643 | Paxs | 376.08 | Joback Method |
| dvisc | 0.0005638 | Paxs | 409.18 | Joback Method |
| dvisc | 0.0004353 | Paxs | 442.28 | Joback Method |
| dvisc | 0.0003484 | Paxs | 475.39 | Joback Method |
| dvisc | 0.0002870 | Paxs | 508.49 | Joback Method |

## 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=C3290060&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3290060&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>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>mccvol:</b>  | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <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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