

# 2,4,6-Trichloro ethyl benzene

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C8H7Cl3/c1-2-6-7(10)3-5(9)4-8(6)11/h3-4H,2H2,1H3 |
| <b>InchiKey:</b>            | MZAUYYMXXORTJT-UHFFFAOYSA-N                               |
| <b>Formula:</b>             | C8H7Cl3   |
| <b>SMILES:</b>              | CCc1c(Cl)cc(Cl)cc1Cl                                      |
| <b>Mol. weight [g/mol]:</b> | 209.50  |
| <b>CAS:</b>                 | 116373-11-6   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 64.21   | kJ/mol  | Joback Method  |
| hf            | -53.55  | kJ/mol  | Joback Method  |
| hfus          | 21.94   | kJ/mol  | Joback Method  |
| hvap          | 50.82   | kJ/mol  | Joback Method  |
| log10ws       | -4.33   |         | Crippen Method |
| logp          | 4.209   |         | Crippen Method |
| mcvol         | 136.540 | ml/mol  | McGowan Method |
| pc            | 3049.04 | kPa     | Joback Method  |
| tb            | 536.35  | K       | Joback Method  |
| tc            | 768.20  | K       | Joback Method  |
| tf            | 333.66  | K       | Joback Method  |
| vc            | 0.522   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 248.30    | J/molxK | 536.35          | Joback Method |
| cpg           | 290.52    | J/molxK | 729.55          | Joback Method |
| cpg           | 283.16    | J/molxK | 690.91          | Joback Method |
| cpg           | 275.28    | J/molxK | 652.27          | Joback Method |
| cpg           | 266.86    | J/molxK | 613.63          | Joback Method |
| cpg           | 257.88    | J/molxK | 574.99          | Joback Method |
| cpg           | 297.38    | J/molxK | 768.20          | Joback Method |
| dvisc         | 0.0002597 | Paxs    | 536.35          | Joback Method |
| dvisc         | 0.0003117 | Paxs    | 502.57          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003841 | Paxs | 468.79 | Joback Method |
| dvisc | 0.0004890 | Paxs | 435.00 | Joback Method |
| dvisc | 0.0006484 | Paxs | 401.22 | Joback Method |
| dvisc | 0.0009054 | Paxs | 367.44 | Joback Method |
| dvisc | 0.0013528 | Paxs | 333.66 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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=C116373116&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116373116&amp;Units=SI</a> |
| <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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>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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