

# triphenylmethane, 3,4-dichloro

**Inchi:** InChI=1S/C19H14Cl2/c20-17-12-11-16(13-18(17)21)19(14-7-3-1-4-8-14)15-9-5-2-6-10-1

**InchiKey:** YPMBTMFUNZQHSY-UHFFFAOYSA-N

**Formula:** C19H14Cl2

**SMILES:** Clc1ccc(C(c2ccccc2)c2ccccc2)cc1Cl

**Mol. weight [g/mol]:** 313.22

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 400.77  | kJ/mol  | Joback Method  |
| hf            | 214.40  | kJ/mol  | Joback Method  |
| hfus          | 31.18   | kJ/mol  | Joback Method  |
| hvap          | 74.42   | kJ/mol  | Joback Method  |
| log10ws       | -6.62   |         | Crippen Method |
| logp          | 6.174   |         | Crippen Method |
| mcvol         | 231.770 | ml/mol  | McGowan Method |
| pc            | 2173.43 | kPa     | Joback Method  |
| rinpol        | 386.30  |         | NIST Webbook   |
| tb            | 798.54  | K       | Joback Method  |
| tc            | 1071.12 | K       | Joback Method  |
| tf            | 453.03  | K       | Joback Method  |
| vc            | 0.868   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 598.30    | J/mol×K | 798.54          | Joback Method |
| cpg           | 613.41    | J/mol×K | 843.97          | Joback Method |
| cpg           | 627.05    | J/mol×K | 889.40          | Joback Method |
| cpg           | 639.36    | J/mol×K | 934.83          | Joback Method |
| cpg           | 650.48    | J/mol×K | 980.26          | Joback Method |
| cpg           | 660.56    | J/mol×K | 1025.69         | Joback Method |
| cpg           | 669.76    | J/mol×K | 1071.12         | Joback Method |
| dvisc         | 0.0009183 | Pa×s    | 453.03          | Joback Method |
| dvisc         | 0.0004956 | Pa×s    | 510.62          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003031 | Pa×s | 568.20 | Joback Method |
| dvisc | 0.0002029 | Pa×s | 625.78 | Joback Method |
| dvisc | 0.0001453 | Pa×s | 683.37 | Joback Method |
| dvisc | 0.0001097 | Pa×s | 740.95 | Joback Method |
| dvisc | 0.0000862 | Pa×s | 798.54 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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.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>                                     |
| <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=R522566&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R522566&amp;Units=SI</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>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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