

# Benzene, 5-chloro-1,2,4-trimethyl

|                      |                                                      |
|----------------------|------------------------------------------------------|
| Inchi:               | InChI=1S/C9H11Cl/c1-6-4-8(3)9(10)5-7(6)2/h4-5H,1-3H3 |
| InchiKey:            | LJQDRBHJSRPHEP-UHFFFAOYSA-N                          |
| Formula:             | C9H11Cl                                              |
| SMILES:              | Cc1cc(C)c(Cl)cc1C                                    |
| Mol. weight [g/mol]: | 154.64                                               |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 96.49   | kJ/mol  | Joback Method  |
| hf            | -42.71  | kJ/mol  | Joback Method  |
| hfus          | 16.14   | kJ/mol  | Joback Method  |
| hvap          | 44.28   | kJ/mol  | Joback Method  |
| log10ws       | -3.58   |         | Crippen Method |
| logp          | 3.265   |         | Crippen Method |
| mcvol         | 126.150 | ml/mol  | McGowan Method |
| pc            | 2976.29 | kPa     | Joback Method  |
| rinpol        | 1177.00 |         | NIST Webbook   |
| rinpol        | 1184.00 |         | NIST Webbook   |
| rinpol        | 1179.00 |         | NIST Webbook   |
| tb            | 484.37  | K       | Joback Method  |
| tc            | 701.99  | K       | Joback Method  |
| tf            | 285.09  | K       | Joback Method  |
| vc            | 0.480   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 243.34 | J/mol×K | 484.37          | Joback Method |
| cpg           | 255.40 | J/mol×K | 520.64          | Joback Method |
| cpg           | 266.86 | J/mol×K | 556.91          | Joback Method |
| cpg           | 277.74 | J/mol×K | 593.18          | Joback Method |
| cpg           | 288.04 | J/mol×K | 629.45          | Joback Method |
| cpg           | 297.78 | J/mol×K | 665.72          | Joback Method |
| cpg           | 306.99 | J/mol×K | 701.99          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0012970 | Pa×s | 285.09 | Joback Method |
| dvisc | 0.0008333 | Pa×s | 318.30 | Joback Method |
| dvisc | 0.0005820 | Pa×s | 351.52 | Joback Method |
| dvisc | 0.0004325 | Pa×s | 384.73 | Joback Method |
| dvisc | 0.0003370 | Pa×s | 417.94 | Joback Method |
| dvisc | 0.0002723 | Pa×s | 451.16 | Joback Method |
| dvisc | 0.0002266 | Pa×s | 484.37 | 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=R132222&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R132222&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.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>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                                 |

Latest version available from:

<https://www.chemeo.com/cid/65-115-2/Benzene-5-chloro-1-2-4-trimethyl.pdf>

Generated by Cheméo on 2025-12-05 19:33:19.395397258 +0000 UTC m=+4711396.925437917.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.