

# Cyclopropane, 1,2,3-trimethyl-

|                      |                                           |
|----------------------|-------------------------------------------|
| Other names:         | 1,2,3-trimethylcyclopropane               |
| Inchi:               | InChI=1S/C6H12/c1-4-5(2)6(4)3/h4-6H,1-3H3 |
| InchiKey:            | PSGQRAAEZLHVDT-UHFFFAOYSA-N               |
| Formula:             | C6H12                                     |
| SMILES:              | CC1C(C)C1C                                |
| Mol. weight [g/mol]: | 84.16                                     |
| CAS:                 | 42984-19-0                                |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 44.97   | kJ/mol  | Joback Method  |
| hf            | -135.05 | kJ/mol  | Joback Method  |
| hfus          | 11.57   | kJ/mol  | Joback Method  |
| hvap          | 28.25   | kJ/mol  | Joback Method  |
| log10ws       | -1.50   |         | Crippen Method |
| logp          | 1.908   |         | Crippen Method |
| mcvol         | 84.540  | ml/mol  | McGowan Method |
| pc            | 3341.24 | kPa     | Joback Method  |
| tb            | 334.08  | K       | Joback Method  |
| tc            | 510.89  | K       | Joback Method  |
| tf            | 166.84  | K       | Joback Method  |
| vc            | 0.327   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 141.35    | J/mol×K | 334.08          | Joback Method |
| cpg           | 198.49    | J/mol×K | 481.42          | Joback Method |
| cpg           | 188.04    | J/mol×K | 451.96          | Joback Method |
| cpg           | 177.11    | J/mol×K | 422.49          | Joback Method |
| cpg           | 165.70    | J/mol×K | 393.02          | Joback Method |
| cpg           | 153.79    | J/mol×K | 363.55          | Joback Method |
| cpg           | 208.48    | J/mol×K | 510.89          | Joback Method |
| dvisc         | 0.0001879 | Pa×s    | 334.08          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001810 | Pa×s | 306.21 | Joback Method |
| dvisc | 0.0001732 | Pa×s | 278.33 | Joback Method |
| dvisc | 0.0001640 | Pa×s | 250.46 | Joback Method |
| dvisc | 0.0001532 | Pa×s | 222.59 | Joback Method |
| dvisc | 0.0001404 | Pa×s | 194.71 | Joback Method |
| dvisc | 0.0001250 | Pa×s | 166.84 | 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=C42984190&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C42984190&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>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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