# Cyclohexane, 1,2,4-trimethyl-, (1«alpha»,2«alpha»,4«beta»)-

**Other names:** 1,cis-2,trans-4-trimethylcyclohexane
cis,trans-1,2,4-trimethylcyclohexane

**Inchi:** InChI=1S/C9H18/c1-7-4-5-8(2)9(3)6-7/h7-9H,4-6H2,1-3H3/t7-,8-,9+/m0/s1

**InchiKey:** VCJPCEVERINRSG-XHNCKOQMSA-N

**Formula:** C9H18

**SMILES:** CC1CCC(C)C(C)C1

**Mol. weight [g/mol]:** 126.24

**CAS:** 7667-58-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 33.93 | kJ/mol | Joback Method |
| hf | -215.45 | kJ/mol | Joback Method |
| hfus | 13.04 | kJ/mol | Joback Method |
| hvap | 35.44 | kJ/mol | Joback Method |
| log10ws | -2.76 | | Crippen Method |
| logp | 3.079 | | Crippen Method |
| mcvol | 126.810 | ml/mol | McGowan Method |
| pc | 2648.83 | kPa | Joback Method |
| rinpol | 861.00 | | NIST Webbook |
| rinpol | 883.30 | | NIST Webbook |
| rinpol | 875.60 | | NIST Webbook |
| rinpol | 861.00 | | NIST Webbook |
| rinpol | 883.30 | | NIST Webbook |
| rinpol | 889.30 | | NIST Webbook |
| rinpol | 893.10 | | NIST Webbook |
| rinpol | 857.00 | | NIST Webbook |
| rinpol | 880.00 | | NIST Webbook |
| rinpol | 890.00 | | NIST Webbook |
| rinpol | 884.00 | | NIST Webbook |
| rinpol | 863.00 | | NIST Webbook |
| rinpol | 886.00 | | NIST Webbook |
| rinpol | 866.00 | | NIST Webbook |
| rinpol | 890.00 | | NIST Webbook |
| rinpol | 870.00 | | NIST Webbook |
| rinpol | 894.00 | | NIST Webbook |
| rinpol | 880.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 875.60 | | NIST Webbook |
| rinpol | 879.40 | | NIST Webbook |
| rinpol | 854.00 | | NIST Webbook |
| rinpol | 854.00 | | NIST Webbook |
| tb | 415.00 ± 3.00 | K | NIST Webbook |
| tc | 613.57 | K | Joback Method |
| tf | 190.09 | K | Joback Method |
| vc | 0.470 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 254.82 | J/mol×K | 415.53 | Joback Method |
| cpg | 273.92 | J/mol×K | 448.54 | Joback Method |
| cpg | 292.21 | J/mol×K | 481.54 | Joback Method |
| cpg | 309.72 | J/mol×K | 514.55 | Joback Method |
| cpg | 326.43 | J/mol×K | 547.56 | Joback Method |
| cpg | 342.37 | J/mol×K | 580.57 | Joback Method |
| cpg | 357.55 | J/mol×K | 613.57 | Joback Method |
| dvisc | 0.0024227 | Pa×s | 190.09 | Joback Method |
| dvisc | 0.0012236 | Pa×s | 227.66 | Joback Method |
| dvisc | 0.0007500 | Pa×s | 265.24 | Joback Method |
| dvisc | 0.0005190 | Pa×s | 302.81 | Joback Method |
| dvisc | 0.0003896 | Pa×s | 340.38 | Joback Method |
| dvisc | 0.0003096 | Pa×s | 377.96 | Joback Method |
| dvisc | 0.0002565 | Pa×s | 415.53 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.49059e+01 |
| Coeff. B | -4.05540e+03 |
| Coeff. C | -2.07950e+01 |
| Temperature range (K), min. | 298.22 |
| Temperature range (K), max. | 443.48 |

# Sources

| | |
|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C7667585&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |