# Phenol, 2,3,5,6-tetramethyl-

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|---|---|
| **Other names:** | 2,3,5,6-Tetramethylphenol |
| | Durenol |
| | Phenol, tetramethyl- |
| **Inchi:** | InChI=1S/C10H14O/c1-6-5-7(2)9(4)10(11)8(6)3/h5,11H,1-4H3 |
| **InchiKey:** | KLAQSPUVCDBEGF-UHFFFAOYSA-N |
| **Formula:** | C10H14O |
| **SMILES:** | Cc1cc(C)c(C)c(O)c1C |
| **Mol. weight [g/mol]:** | 150.22 |
| **CAS:** | 527-35-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -37.78 | kJ/mol | Joback Method |
| hf | -224.92 | kJ/mol | Joback Method |
| hfus | 20.31 | kJ/mol | Joback Method |
| hvap | 55.13 | kJ/mol | Joback Method |
| log10ws | -2.92 | | Crippen Method |
| logp | 2.626 | | Crippen Method |
| mcvol | 133.870 | ml/mol | McGowan Method |
| pc | 3291.59 | kPa | Joback Method |
| rinpol | 1287.00 | | NIST Webbook |
| rinpol | 1354.00 | | NIST Webbook |
| rinpol | 231.30 | | NIST Webbook |
| rinpol | 1361.00 | | NIST Webbook |
| rinpol | 232.59 | | NIST Webbook |
| rinpol | 1319.00 | | NIST Webbook |
| rinpol | 1319.00 | | NIST Webbook |
| rinpol | 231.30 | | NIST Webbook |
| rinpol | 1354.00 | | NIST Webbook |
| tb | 520.70 ± 4.00 | K | NIST Webbook |
| tb | 522.00 ± 3.00 | K | NIST Webbook |
| tb | 520.70 ± 4.00 | K | NIST Webbook |
| tc | 772.15 | K | Joback Method |
| tf | 392.00 ± 2.00 | K | NIST Webbook |
| tf | 390.00 ± 2.00 | K | NIST Webbook |
| tf | 390.00 ± 2.00 | K | NIST Webbook |
| tf | 392.00 ± 2.00 | K | NIST Webbook |

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|---|---|---|---|
| tf | 389.00 ± 3.00 | K | NIST Webbook |
| vc | 0.454 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 310.51 | J/mol×K | 550.44 | Joback Method |
| cpg | 323.33 | J/mol×K | 587.39 | Joback Method |
| cpg | 335.42 | J/mol×K | 624.34 | Joback Method |
| cpg | 346.83 | J/mol×K | 661.30 | Joback Method |
| cpg | 357.63 | J/mol×K | 698.25 | Joback Method |
| cpg | 367.86 | J/mol×K | 735.20 | Joback Method |
| cpg | 377.60 | J/mol×K | 772.15 | Joback Method |
| dvisc | 0.0010235 | Pa×s | 378.16 | Joback Method |
| dvisc | 0.0005185 | Pa×s | 406.87 | Joback Method |
| dvisc | 0.0002873 | Pa×s | 435.59 | Joback Method |
| dvisc | 0.0001712 | Pa×s | 464.30 | Joback Method |
| dvisc | 0.0001084 | Pa×s | 493.01 | Joback Method |
| dvisc | 0.0000722 | Pa×s | 521.73 | Joback Method |
| dvisc | 0.0000501 | Pa×s | 550.44 | Joback Method |
| hvapt | 51.20 | kJ/mol | 451.50 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.54956e+01 |
| Coeff. B | -4.72801e+03 |
| Coeff. C | -8.60300e+01 |
| Temperature range (K), min. | 390.15 |
| Temperature range (K), max. | 550.28 |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C527355&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 |
| **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 |

# 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 |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **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 |