# Benzenemethanol, «alpha»,«alpha»-dimethyl-

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|---|---|
| **Other names:** | 1-Hydroxycumene |
| | 1-Methyl-1-phenylethanol |
| | 2-Hydroxy-2-phenylpropane |
| | 2-Phenyl-2-propanol |
| | 2-Phenylisopropanol |
| | 2-Propanol, 2-phenyl- |
| | 2-phenylpropan-2-ol |
| | Benzenemethanol, .alpha.,.alpha.-dimethyl- |
| | Benzyl alcohol, «alpha»,«alpha»-dimethyl- |
| | Benzyl alcohol, Â«alphaÂ»,Â«alphaÂ»-dimethyl- |
| | Dimethyl phenyl carbinol |
| | Dimethylphenylcarbinol |
| | Dimethylphenylmethanol |
| | NSC 1261 |
| | NSC 212537 |
| | Phenyldimethylcarbinol |
| | «alpha»,«alpha»-Dimethylbenzenemethanol |
| | «alpha»,«alpha»-Dimethylbenzyl alcohol |
| | «alpha»-Cumyl alcohol |
| | Â«alphaÂ»,Â«alphaÂ»-Dimethylbenzenemethanol |
| | Â«alphaÂ»,Â«alphaÂ»-Dimethylbenzyl alcohol |
| | Â«alphaÂ»-Cumyl alcohol |
| **Inchi:** | InChI=1S/C9H12O/c1-9(2,10)8-6-4-3-5-7-8/h3-7,10H,1-2H3 |
| **InchiKey:** | BDCFWIDZNLCTMF-UHFFFAOYSA-N |
| **Formula:** | C9H12O |
| **SMILES:** | CC(C)(O)c1ccccc1 |
| **Mol. weight [g/mol]:** | 136.19 |
| **CAS:** | 617-94-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -5006.20 ± 2.20 | kJ/mol | NIST Webbook |
| gf | 3.33 | kJ/mol | Joback Method |
| hf | -153.54 | kJ/mol | Joback Method |
| hfs | -250.40 ± 2.30 | kJ/mol | NIST Webbook |
| hfus | 9.78 | kJ/mol | Joback Method |

| | | | |
|---|---|---|---|
| hsub | 82.30 ± 0.70 | kJ/mol | NIST Webbook |
| hvap | 65.00 ± 0.50 | kJ/mol | NIST Webbook |
| log10ws | -2.13 | | Crippen Method |
| logp | 1.914 | | Crippen Method |
| mcvol | 119.780 | ml/mol | McGowan Method |
| pc | 3718.02 | kPa | Joback Method |
| rinpol | 1098.00 | | NIST Webbook |
| rinpol | 1089.60 | | NIST Webbook |
| rinpol | 1089.00 | | NIST Webbook |
| rinpol | 1090.00 | | NIST Webbook |
| rinpol | 1090.00 | | NIST Webbook |
| rinpol | 1080.00 | | NIST Webbook |
| rinpol | 1057.00 | | NIST Webbook |
| rinpol | 1076.00 | | NIST Webbook |
| rinpol | 1095.00 | | NIST Webbook |
| rinpol | 1076.00 | | NIST Webbook |
| rinpol | 1098.00 | | NIST Webbook |
| rinpol | 1057.00 | | NIST Webbook |
| rinpol | 1098.00 | | NIST Webbook |
| rinpol | 1102.00 | | NIST Webbook |
| ripol | 1776.00 | | NIST Webbook |
| ripol | 1782.00 | | NIST Webbook |
| ripol | 1770.00 | | NIST Webbook |
| ripol | 1759.00 | | NIST Webbook |
| ripol | 1779.00 | | NIST Webbook |
| ripol | 1770.00 | | NIST Webbook |
| ripol | 1770.00 | | NIST Webbook |
| tb | 475.20 | K | NIST Webbook |
| tc | 728.04 | K | Joback Method |
| tf | 346.00 ± 3.00 | K | NIST Webbook |
| tf | 310.00 ± 1.00 | K | NIST Webbook |
| vc | 0.440 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 324.80 | J/mol×K | 693.52 | Joback Method |
| cpg | 333.56 | J/mol×K | 728.04 | Joback Method |
| cpg | 270.14 | J/mol×K | 520.95 | Joback Method |
| cpg | 282.69 | J/mol×K | 555.46 | Joback Method |
| cpg | 294.38 | J/mol×K | 589.98 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 305.26 | J/mol×K | 624.49 | Joback Method |
| cpg | 315.39 | J/mol×K | 659.01 | Joback Method |
| dvisc | 0.0001992 | Pa×s | 480.93 | Joback Method |
| dvisc | 0.0001204 | Pa×s | 520.95 | Joback Method |
| dvisc | 0.0212186 | Pa×s | 280.85 | Joback Method |
| dvisc | 0.0052355 | Pa×s | 320.87 | Joback Method |
| dvisc | 0.0017619 | Pa×s | 360.88 | Joback Method |
| dvisc | 0.0007369 | Pa×s | 400.90 | Joback Method |
| dvisc | 0.0003611 | Pa×s | 440.92 | Joback Method |
| hsubt | 87.50 ± 2.60 | kJ/mol | 294.00 | NIST Webbook |
| hsubt | 82.80 ± 0.70 | kJ/mol | 289.00 | NIST Webbook |
| hvapt | 52.90 | kJ/mol | 407.00 | NIST Webbook |
| hvapt | 63.40 ± 0.50 | kJ/mol | 324.50 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.64941e+01 |
| Coeff. B | -5.17060e+03 |
| Coeff. C | -3.97590e+01 |
| Temperature range (K), min. | 358.80 |
| Temperature range (K), max. | 502.14 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 1.07927e+02 |
| Coeff. B | -1.09574e+04 |
| Coeff. C | -1.32851e+01 |
| Coeff. D | 7.56204e-06 |
| Temperature range (K), min. | 379.15 |
| Temperature range (K), max. | 431.15 |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C617947&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **KDB Vapor Pressure Data:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=882 |
| **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 |
| **KDB:** | https://www.cheric.org/files/research/kdb/mol/mol882.mol |

# Legend

| | |
|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfs:** | Solid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hsub:** | Enthalpy of sublimation at standard conditions |
| **hsubt:** | Enthalpy of sublimation at a given temperature |
| **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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |