# Phenol, 3,5-dimethyl-

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|---|---|
| **Other names:** | 1,3,5-Xylenol |
| | 1,3-Dimethyl-5-hydroxybenzene |
| | 1,5-Dimethyl-3-hydroxybenzene |
| | 1-HYDROXY-3,5-DIMETHYLBENZENE |
| | 3,5-DIMETHYLPHENOL |
| | 3,5-Dmp |
| | 3,5-Xylen-1-ol |
| | 3,5-Xylenol |
| | NSC 9268 |
| | benzene, 1-hydroxy-3,5-dimethyl- |
| **Inchi:** | InChI=1S/C8H10O/c1-6-3-7(2)5-8(9)4-6/h3-5,9H,1-2H3 |
| **InchiKey:** | TUAMRELNJMMDMT-UHFFFAOYSA-N |
| **Formula:** | C8H10O |
| **SMILES:** | Cc1cc(C)cc(O)c1 |
| **Mol. weight [g/mol]:** | 122.16 |
| **CAS:** | 108-68-9 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -4332.80 ± 1.20 | kJ/mol | NIST Webbook |
| dm | 1.80 | debye | KDB |
| gf | -35.36 | kJ/mol | Joback Method |
| hf | -161.60 ± 0.67 | kJ/mol | NIST Webbook |
| hf | -161.50 | kJ/mol | KDB |
| hfs | -244.50 ± 1.20 | kJ/mol | NIST Webbook |
| hfus | 15.91 | kJ/mol | Joback Method |
| hsub | 82.80 ± 0.30 | kJ/mol | NIST Webbook |
| hsub | 82.90 | kJ/mol | NIST Webbook |
| hvap | 45.40 | kJ/mol | NIST Webbook |
| hvap | 82.01 | kJ/mol | NIST Webbook |
| log10ws | -1.40 | | Estimated Solubility Method |
| log10ws | -1.40 | | Aqueous Solubility Prediction Method |
| logp | 2.009 | | Crippen Method |
| mcvol | 105.690 | ml/mol | McGowan Method |
| pc | 5572.87 ± 303.98 | kPa | NIST Webbook |

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|---|---|---|
| rinpol | 1179.00 | NIST Webbook |
| rinpol | 196.53 | NIST Webbook |
| rinpol | 1143.00 | NIST Webbook |
| rinpol | 1179.00 | NIST Webbook |
| rinpol | 193.40 | NIST Webbook |
| rinpol | 1143.00 | NIST Webbook |
| rinpol | 1146.00 | NIST Webbook |
| rinpol | 1139.00 | NIST Webbook |
| rinpol | 1139.00 | NIST Webbook |
| rinpol | 1146.00 | NIST Webbook |
| rinpol | 1173.00 | NIST Webbook |
| rinpol | 1124.00 | NIST Webbook |
| rinpol | 1163.00 | NIST Webbook |
| rinpol | 1143.40 | NIST Webbook |
| rinpol | 1187.00 | NIST Webbook |
| rinpol | 1169.50 | NIST Webbook |
| rinpol | 1170.00 | NIST Webbook |
| rinpol | 1171.30 | NIST Webbook |
| rinpol | 1171.00 | NIST Webbook |
| rinpol | 1147.00 | NIST Webbook |
| rinpol | 1168.00 | NIST Webbook |
| rinpol | 1196.00 | NIST Webbook |
| rinpol | 1181.00 | NIST Webbook |
| rinpol | 1165.00 | NIST Webbook |
| rinpol | 1170.00 | NIST Webbook |
| rinpol | 1141.00 | NIST Webbook |
| rinpol | 1143.00 | NIST Webbook |
| rinpol | 1144.00 | NIST Webbook |
| rinpol | 1139.00 | NIST Webbook |
| rinpol | 1173.00 | NIST Webbook |
| rinpol | 196.48 | NIST Webbook |
| rinpol | 1167.00 | NIST Webbook |
| rinpol | 1145.00 | NIST Webbook |
| rinpol | 1163.00 | NIST Webbook |
| rinpol | 1187.00 | NIST Webbook |
| rinpol | 1193.00 | NIST Webbook |
| rinpol | 1194.00 | NIST Webbook |
| rinpol | 1169.00 | NIST Webbook |
| rinpol | 1178.00 | NIST Webbook |
| ripol | 2163.00 | NIST Webbook |
| ripol | 2174.00 | NIST Webbook |
| ripol | 2181.00 | NIST Webbook |
| ripol | 2146.00 | NIST Webbook |
| ripol | 2105.00 | NIST Webbook |

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|---|---|---|---|
| ripol | 2105.00 | | NIST Webbook |
| ripol | 2174.00 | | NIST Webbook |
| tb | 494.89 | K | KDB |
| tc | 766.15 ± 2.00 | K | NIST Webbook |
| tc | 715.60 | K | KDB |
| tc | 715.55 ± 0.80 | K | NIST Webbook |
| tf | 336.75 | K | Aqueous Solubility Prediction Method |
| tf | 336.70 | K | KDB |
| tf | 336.92 | K | (Solid + liquid) phase equilibria and solid-compound formation in (N-methyl-2-pyrrolidinone + phenol, or 3,5-dimethylphenol) |
| vc | 0.342 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 224.69 | J/mol×K | 494.72 | Joback Method |
| cpg | 236.18 | J/mol×K | 532.60 | Joback Method |
| cpg | 246.85 | J/mol×K | 570.49 | Joback Method |
| cpg | 256.78 | J/mol×K | 608.37 | Joback Method |
| cpg | 266.04 | J/mol×K | 646.26 | Joback Method |
| cpg | 274.69 | J/mol×K | 684.14 | Joback Method |
| cpg | 282.81 | J/mol×K | 722.03 | Joback Method |
| dvisc | 0.0000891 | Pa×s | 494.72 | Joback Method |
| dvisc | 0.0013928 | Pa×s | 357.94 | Joback Method |
| dvisc | 0.0006876 | Pa×s | 385.29 | Joback Method |
| dvisc | 0.0003727 | Pa×s | 412.65 | Joback Method |
| dvisc | 0.0031710 | Pa×s | 330.58 | Joback Method |
| dvisc | 0.0001358 | Pa×s | 467.36 | Joback Method |
| dvisc | 0.0002180 | Pa×s | 440.01 | Joback Method |
| hfust | 18.00 | kJ/mol | 336.80 | NIST Webbook |
| hfust | 17.42 | kJ/mol | 336.59 | NIST Webbook |
| hfust | 18.00 | kJ/mol | 336.80 | NIST Webbook |
| hfust | 18.00 | kJ/mol | 336.80 | NIST Webbook |
| hsubt | 82.80 ± 0.30 | kJ/mol | 302.50 | NIST Webbook |
| hsubt | 63.20 ± 0.80 | kJ/mol | 299.00 | NIST Webbook |
| hvapt | 55.30 | kJ/mol | 462.00 | NIST Webbook |
| sfust | 53.38 | J/mol×K | 336.80 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.55172e+01 |
| Coeff. B | -4.52595e+03 |
| Coeff. C | -7.87290e+01 |
| Temperature range (K), min. | 375.91 |
| Temperature range (K), max. | 522.20 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 1.56615e+02 |
| Coeff. B | -1.41866e+04 |
| Coeff. C | -2.01992e+01 |
| Coeff. D | 8.12303e-06 |
| Temperature range (K), min. | 336.59 |
| Temperature range (K), max. | 715.65 |

# Sources

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|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **(Solid + liquid) phase equilibria and solid-compound formation in (N-methyl-2-pyrrolidinone + phenol, or 3,5-dimethylphenol):** | https://www.doi.org/10.1016/j.fluid.2005.03.027 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C108689&Units=SI |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **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 |
| **Estimated Solubility Method:** | http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| **KDB Vapor Pressure Data:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=879 |
| **Experiments and COSMO-SAC Modeling of Methyl Isobutyl Ketone + Dimethylphenols + Water Mixtures:** | https://www.doi.org/10.1021/acs.jced.9b00300 |
| **KDB:** | https://www.cheric.org/files/research/kdb/mol/mol879.mol |

# Legend

| | |
|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **dm:** | Dipole Moment |
| **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 |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **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 |
| **sfust:** | Entropy of fusion at a given temperature |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |