# Phenol, 3-(1-methylethyl)-

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|---|---|
| **Other names:** | 3-(1-Methylethyl)phenol |
| | 3-Isopropylphenol |
| | 3-isopropylhydroxybenzene |
| | Isopropylphenol, meta |
| | Phenol, m-isopropyl- |
| | m-Cumenol |
| | m-Isopropylphenol |
| **Inchi:** | InChI=1S/C9H12O/c1-7(2)8-4-3-5-9(10)6-8/h3-7,10H,1-2H3 |
| **InchiKey:** | VLJSLTNSFSOYQR-UHFFFAOYSA-N |
| **Formula:** | C9H12O |
| **SMILES:** | CC(C)c1cccc(O)c1 |
| **Mol. weight [g/mol]:** | 136.19 |
| **CAS:** | 618-45-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -4993.60 | kJ/mol | NIST Webbook |
| gf | -19.75 | kJ/mol | Joback Method |
| hf | -175.30 ± 2.40 | kJ/mol | NIST Webbook |
| hf | -190.60 | kJ/mol | NIST Webbook |
| hfl | -260.00 | kJ/mol | NIST Webbook |
| hfus | 15.37 | kJ/mol | Joback Method |
| hvap | 69.40 | kJ/mol | NIST Webbook |
| hvap | 73.01 | kJ/mol | NIST Webbook |
| log10ws | -2.20 | | Crippen Method |
| logp | 2.516 | | Crippen Method |
| mcvol | 119.780 | ml/mol | McGowan Method |
| pc | 3935.71 | kPa | Joback Method |
| rinpol | 1227.30 | | NIST Webbook |
| rinpol | 1207.00 | | NIST Webbook |
| rinpol | 1228.00 | | NIST Webbook |
| rinpol | 1229.20 | | NIST Webbook |
| rinpol | 1227.90 | | NIST Webbook |
| rinpol | 1207.00 | | NIST Webbook |
| tb | 512.18 | K | Joback Method |
| tc | 739.56 | K | Joback Method |
| tf | 299.15 ± 2.00 | K | NIST Webbook |

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|---|---|---|---|
| tf | 299.15 ± 2.00 | K | NIST Webbook |
| tf | 299.15 ± 2.00 | K | NIST Webbook |
| tf | 299.15 ± 2.00 | K | NIST Webbook |
| tf | 298.85 ± 0.20 | K | NIST Webbook |
| tf | 299.15 ± 2.00 | K | NIST Webbook |
| vc | 0.392 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 267.53 | J/mol×K | 512.18 | Joback Method |
| cpg | 280.87 | J/mol×K | 550.08 | Joback Method |
| cpg | 293.23 | J/mol×K | 587.97 | Joback Method |
| cpg | 304.71 | J/mol×K | 625.87 | Joback Method |
| cpg | 315.38 | J/mol×K | 663.76 | Joback Method |
| cpg | 325.34 | J/mol×K | 701.66 | Joback Method |
| cpg | 334.65 | J/mol×K | 739.56 | Joback Method |
| dvisc | 0.0072081 | Pa×s | 314.33 | Joback Method |
| dvisc | 0.0023278 | Pa×s | 347.31 | Joback Method |
| dvisc | 0.0009146 | Pa×s | 380.28 | Joback Method |
| dvisc | 0.0004171 | Pa×s | 413.25 | Joback Method |
| dvisc | 0.0002136 | Pa×s | 446.23 | Joback Method |
| dvisc | 0.0001200 | Pa×s | 479.21 | Joback Method |
| dvisc | 0.0000726 | Pa×s | 512.18 | Joback Method |
| hvapt | 64.30 | kJ/mol | 437.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.54407e+01 |
| Coeff. B | -4.55275e+03 |
| Coeff. C | -8.04700e+01 |
| Temperature range (K), min. | 380.92 |
| Temperature range (K), max. | 529.94 |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C618451&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 |

# Legend

| | |
|---|---|
| **chl:** | Standard liquid 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 |
| **hfl:** | Liquid phase 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 |