# Phenol, 4-(1-methylpropyl)-

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|---|---|
| **Other names:** | 1-Hydroxy-4-sec-butylbenzene |
| | 4-(1-Methylpropyl)phenol |
| | 4-(2-Butyl)phenol |
| | 4-sec-Butylphenol |
| | Phenol, p-sec-butyl- |
| | p-(1-Methylpropyl)phenol |
| | p-sec-Butylphenol |
| **Inchi:** | InChI=1S/C10H14O/c1-3-8(2)9-4-6-10(11)7-5-9/h4-8,11H,3H2,1-2H3 |
| **InchiKey:** | ZUTYZAFDFLLILI-UHFFFAOYSA-N |
| **Formula:** | C10H14O |
| **SMILES:** | CCC(C)c1ccc(O)cc1 |
| **Mol. weight [g/mol]:** | 150.22 |
| **CAS:** | 99-71-8 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -11.33 | kJ/mol | Joback Method |
| hf | -190.30 | kJ/mol | NIST Webbook |
| hfl | -256.40 | kJ/mol | NIST Webbook |
| hfus | 17.96 | kJ/mol | Joback Method |
| hvap | 66.10 | kJ/mol | NIST Webbook |
| log10ws | -2.62 | | Crippen Method |
| logp | 2.906 | | Crippen Method |
| mcvol | 133.870 | ml/mol | McGowan Method |
| pc | 3501.28 | kPa | Joback Method |
| rinpol | 1313.70 | | NIST Webbook |
| rinpol | 1279.00 | | NIST Webbook |
| rinpol | 1279.00 | | NIST Webbook |
| rinpol | 1265.00 | | NIST Webbook |
| rinpol | 1285.00 | | NIST Webbook |
| rinpol | 1317.90 | | NIST Webbook |
| rinpol | 1315.30 | | NIST Webbook |
| rinpol | 1293.00 | | NIST Webbook |
| rinpol | 1265.00 | | NIST Webbook |
| ripol | 2068.00 | | NIST Webbook |
| ripol | 2068.00 | | NIST Webbook |
| tb | 535.06 | K | Joback Method |

| | | | |
|---|---|---|---|
| tc | 758.39 | K | Joback Method |
| tf | 335.15 ± 2.00 | K | NIST Webbook |
| tf | 327.15 ± 6.00 | K | NIST Webbook |
| tf | 332.15 ± 2.00 | K | NIST Webbook |
| tf | 332.15 ± 3.00 | K | NIST Webbook |
| tf | 334.65 ± 2.00 | K | NIST Webbook |
| tf | 334.65 ± 2.00 | K | NIST Webbook |
| tf | 325.15 ± 6.00 | K | NIST Webbook |
| tf | 332.40 ± 4.00 | K | NIST Webbook |
| tf | 332.15 ± 2.00 | K | NIST Webbook |
| tf | 331.40 ± 2.00 | K | NIST Webbook |
| tf | 327.65 ± 5.00 | K | NIST Webbook |
| tf | 326.65 ± 5.00 | K | NIST Webbook |
| vc | 0.448 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 311.88 | J/mol×K | 535.06 | Joback Method |
| cpg | 326.10 | J/mol×K | 572.28 | Joback Method |
| cpg | 339.34 | J/mol×K | 609.50 | Joback Method |
| cpg | 351.67 | J/mol×K | 646.73 | Joback Method |
| cpg | 363.20 | J/mol×K | 683.95 | Joback Method |
| cpg | 373.98 | J/mol×K | 721.17 | Joback Method |
| cpg | 384.11 | J/mol×K | 758.39 | Joback Method |
| dvisc | 0.0057625 | Pa×s | 325.60 | Joback Method |
| dvisc | 0.0018414 | Pa×s | 360.51 | Joback Method |
| dvisc | 0.0007197 | Pa×s | 395.42 | Joback Method |
| dvisc | 0.0003276 | Pa×s | 430.33 | Joback Method |
| dvisc | 0.0001678 | Pa×s | 465.24 | Joback Method |
| dvisc | 0.0000944 | Pa×s | 500.15 | Joback Method |
| dvisc | 0.0000572 | Pa×s | 535.06 | Joback Method |
| hvapt | 59.00 | kJ/mol | 430.00 | NIST Webbook |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 408.70 | K | 3.30 | NIST Webbook |

| | | | | |
|---|---|---|---|---|
| tbrp | 402.00 ± 1.00 | K | 2.40 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.54517e+01 |
| Coeff. B | -4.66767e+03 |
| Coeff. C | -8.43890e+01 |
| Temperature range (K), min. | 392.20 |
| Temperature range (K), max. | 544.70 |

# Sources

**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=C99718&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

# Legend

**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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |