# BENZENEBUTANOL

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|---|---|
| **Other names:** | 1-butanol, 4-phenyl- |
| | 4-Phenyl butanol-1 |
| | 4-Phenyl-n-butanol |
| | 4-Phenylbutanol |
| | 4-phenyl-1-butanol |
| | 4-phenylbutan-1-ol |
| | Phenylbutyl alcohol |
| **Inchi:** | InChI=1S/C10H14O/c11-9-5-4-8-10-6-2-1-3-7-10/h1-3,6-7,11H,4-5,8-9H2 |
| **InchiKey:** | LDZLXQFDGRCELX-UHFFFAOYSA-N |
| **Formula:** | C10H14O |
| **SMILES:** | OCCCCc1ccccc1 |
| **Mol. weight [g/mol]:** | 150.22 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.6853 | | Cheméo Relay (1.0) |
| gf | 8.91 | kJ/mol | Joback Method |
| hf | -159.85 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 19.79 | kJ/mol | Joback Method |
| hvap | 83.75 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.81 | eV | Cheméo Relay (1.0) |
| log10ws | -1.70 | | Cheméo Relay (1.0) |
| logp | 2.002 | | Crippen Method |
| mcvol | 133.870 | ml/mol | McGowan Method |
| pc | 3070.00 | kPa | Vapor-Liquid Critical Properties of Phenol and (C8 to C10) Phenylalkanols |
| tb | 539.60 | K | Cheméo Relay (1.0) |
| tc | 756.86 | K | Cheméo Relay (1.0) |
| tf | 258.57 | K | Cheméo Relay (1.0) |
| vc | 0.483 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 311.72 | J/mol×K | 547.06 | Joback Method |
| cpg | 324.22 | J/mol×K | 579.13 | Joback Method |
| cpg | 336.04 | J/mol×K | 611.20 | Joback Method |
| cpg | 347.19 | J/mol×K | 643.27 | Joback Method |
| cpg | 357.73 | J/mol×K | 675.33 | Joback Method |
| cpg | 367.66 | J/mol×K | 707.40 | Joback Method |
| cpg | 377.01 | J/mol×K | 739.47 | Joback Method |
| dvisc | 0.0140109 | Pa×s | 289.70 | Joback Method |
| dvisc | 0.0036769 | Pa×s | 332.59 | Joback Method |
| dvisc | 0.0013099 | Pa×s | 375.49 | Joback Method |
| dvisc | 0.0005766 | Pa×s | 418.38 | Joback Method |
| dvisc | 0.0002957 | Pa×s | 461.27 | Joback Method |
| dvisc | 0.0001699 | Pa×s | 504.17 | Joback Method |
| dvisc | 0.0001065 | Pa×s | 547.06 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 413.20 | K | 1.90 | NIST Webbook |

# Sources

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C3360416&Units=SI

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Vapor-Liquid Critical Properties of Phenol and (C8 to C10) Phenylalkanols:** https://www.doi.org/10.1021/je0604380

**Partitioning of Phenylalkanols between Micelles and Water Studied by Limiting Interdiffusion Coefficients in Water and Tetradecyltrimethylammonium Bromide Solutions:** https://www.doi.org/10.1021/je900967j

# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **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 |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |