# Benzene, 1,1'-(1,4-butanediyl)bis-

**Other names:** 1,4-Diphenyl-n-butane
1,4-Diphenylbutane
Butane, 1,4-diphenyl-
**Inchi:** InChI=1S/C16H18/c1-3-9-15(10-4-1)13-7-8-14-16-11-5-2-6-12-16/h1-6,9-12H,7-8,13-14H
**InchiKey:** GLJFYGFBITUZOE-UHFFFAOYSA-N
**Formula:** C16H18
**SMILES:** c1ccc(CCCCc2ccccc2)cc1
**Mol. weight [g/mol]:** 210.31
**CAS:** 1083-56-3

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 822.00 | kJ/mol | NIST Webbook |
| basg | 779.80 | kJ/mol | NIST Webbook |
| chs | -8858.70 ± 2.00 | kJ/mol | NIST Webbook |
| chs | -9121.10 | kJ/mol | NIST Webbook |
| chs | -8912.00 | kJ/mol | NIST Webbook |
| gf | 308.66 | kJ/mol | Joback Method |
| hf | 99.49 | kJ/mol | Joback Method |
| hfus | 25.28 | kJ/mol | Joback Method |
| hvap | 55.76 | kJ/mol | Joback Method |
| log10ws | -4.73 | | Crippen Method |
| logp | 4.252 | | Crippen Method |
| mcvol | 188.780 | ml/mol | McGowan Method |
| pc | 2284.95 | kPa | Joback Method |
| rinpol | 1793.00 | | NIST Webbook |
| rinpol | 1742.90 | | NIST Webbook |
| rinpol | 1780.00 | | NIST Webbook |
| rinpol | 1756.00 | | NIST Webbook |
| rinpol | 1756.00 | | NIST Webbook |
| rinpol | 1780.00 | | NIST Webbook |
| ripol | 2398.00 | | NIST Webbook |
| ripol | 2355.00 | | NIST Webbook |
| ripol | 2398.00 | | NIST Webbook |
| tb | 589.06 ± 0.20 | K | NIST Webbook |
| tb | 590.20 | K | NIST Webbook |
| tc | 848.87 | K | Joback Method |

| | | | |
|---|---|---|---|
| tf | 325.70 ± 0.40 | K | NIST Webbook |
| tf | 325.00 ± 2.00 | K | NIST Webbook |
| tf | 325.70 ± 1.50 | K | NIST Webbook |
| tf | 325.00 ± 3.00 | K | NIST Webbook |
| tf | 325.40 ± 4.00 | K | NIST Webbook |
| tf | 326.00 ± 3.00 | K | NIST Webbook |
| tf | 325.42 ± 0.10 | K | NIST Webbook |
| tf | 330.00 ± 4.00 | K | NIST Webbook |
| tf | 326.00 ± 3.00 | K | NIST Webbook |
| vc | 0.716 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 472.31 | J/mol×K | 618.84 | Joback Method |
| cpg | 553.12 | J/mol×K | 810.54 | Joback Method |
| cpg | 539.32 | J/mol×K | 772.20 | Joback Method |
| cpg | 524.42 | J/mol×K | 733.86 | Joback Method |
| cpg | 508.34 | J/mol×K | 695.52 | Joback Method |
| cpg | 490.99 | J/mol×K | 657.18 | Joback Method |
| cpg | 565.89 | J/mol×K | 848.87 | Joback Method |
| dvisc | 0.0001505 | Pa×s | 618.84 | Joback Method |
| dvisc | 0.0001960 | Pa×s | 569.52 | Joback Method |
| dvisc | 0.0002681 | Pa×s | 520.20 | Joback Method |
| dvisc | 0.0003918 | Pa×s | 470.88 | Joback Method |
| dvisc | 0.0006257 | Pa×s | 421.56 | Joback Method |
| dvisc | 0.0011311 | Pa×s | 372.24 | Joback Method |
| dvisc | 0.0024502 | Pa×s | 322.92 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.43669e+01 |
| Coeff. B | -4.72796e+03 |
| Coeff. C | -1.05212e+02 |
| Temperature range (K), min. | 441.02 |

| | |
|---|---|
| Temperature range (K), max. | 627.32 |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1083563&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

| | |
|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **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 |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **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 |