# Benzene, 1,1'-[oxybis(methylene)]bis-

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|---|---|
| **Other names:** | BA |
| | BA (Plasticizer) |
| | BENZYL ETHER |
| | BENZYL OXIDE |
| | Dibenzyl Ether |
| | Plastikator BA |
| | benzene, 1,1'-[oxybis(methylene)]-bis- |
| | bis(phenylmethyl) ether |
| **Inchi:** | InChI=1S/C14H14O/c1-3-7-13(8-4-1)11-15-12-14-9-5-2-6-10-14/h1-10H,11-12H2 |
| **InchiKey:** | MHDVGSVTJDSBDK-UHFFFAOYSA-N |
| **Formula:** | C14H14O |
| **SMILES:** | c1ccc(COCc2ccccc2)cc1 |
| **Mol. weight [g/mol]:** | 198.26 |
| **CAS:** | 103-50-4 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 186.82 | kJ/mol | Joback Method |
| hf | 8.55 | kJ/mol | Joback Method |
| hfus | 21.29 | kJ/mol | Joback Method |
| hvap | 53.72 | kJ/mol | Joback Method |
| ie | 9.17 | eV | NIST Webbook |
| ie | 8.50 | eV | NIST Webbook |
| log10ws | -3.97 | | Crippen Method |
| logp | 3.403 | | Crippen Method |
| mcvol | 166.470 | ml/mol | McGowan Method |
| nfpaf | %!d(float64=1) | | KDB |
| pc | 2721.17 | kPa | Joback Method |
| rinpol | 1641.40 | | NIST Webbook |
| rinpol | 1649.70 | | NIST Webbook |
| rinpol | 1669.00 | | NIST Webbook |
| rinpol | 1670.00 | | NIST Webbook |
| rinpol | 1676.00 | | NIST Webbook |
| rinpol | 1676.00 | | NIST Webbook |
| rinpol | 1631.00 | | NIST Webbook |
| rinpol | 1616.00 | | NIST Webbook |
| rinpol | 1656.90 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 281.19 | | NIST Webbook |
| rinpol | 1669.00 | | NIST Webbook |
| rinpol | 1616.20 | | NIST Webbook |
| rinpol | 1650.30 | | NIST Webbook |
| rinpol | 1650.30 | | NIST Webbook |
| rinpol | 1650.30 | | NIST Webbook |
| rinpol | 1649.70 | | NIST Webbook |
| rinpol | 1641.40 | | NIST Webbook |
| rinpol | 1620.20 | | NIST Webbook |
| rinpol | 1656.90 | | NIST Webbook |
| rinpol | 1650.30 | | NIST Webbook |
| rinpol | 1620.00 | | NIST Webbook |
| ripol | 2356.00 | | NIST Webbook |
| ripol | 2323.00 | | NIST Webbook |
| tb | 571.20 | K | NIST Webbook |
| tb | 273.15 ± 3.00 | K | NIST Webbook |
| tc | 831.56 | K | Joback Method |
| tf | 293.00 ± 2.00 | K | NIST Webbook |
| vc | 0.622 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 398.13 | J/mol×K | 595.50 | Joback Method |
| cpg | 415.33 | J/mol×K | 634.84 | Joback Method |
| cpg | 431.28 | J/mol×K | 674.19 | Joback Method |
| cpg | 446.05 | J/mol×K | 713.53 | Joback Method |
| cpg | 459.69 | J/mol×K | 752.87 | Joback Method |
| cpg | 472.26 | J/mol×K | 792.21 | Joback Method |
| cpg | 483.81 | J/mol×K | 831.56 | Joback Method |
| dvisc | 0.0005545 | Pa×s | 413.57 | Joback Method |
| dvisc | 0.0009544 | Pa×s | 368.09 | Joback Method |
| dvisc | 0.0019145 | Pa×s | 322.61 | Joback Method |
| dvisc | 0.0003587 | Pa×s | 459.06 | Joback Method |
| dvisc | 0.0002510 | Pa×s | 504.54 | Joback Method |
| dvisc | 0.0001864 | Pa×s | 550.02 | Joback Method |
| dvisc | 0.0001448 | Pa×s | 595.50 | Joback Method |
| hvapt | 45.60 | kJ/mol | 346.00 | NIST Webbook |
| hvapt | 59.40 | kJ/mol | 437.00 | NIST Webbook |

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|---|---|---|---|---|
| rhol | 1039.32 | kg/m3 | 298.00 | Optimization of liquid-liquid equilibria of the type 2 ternary systems (water + valeric acid + aromatic solvent): Modeling through SERLAS |
| rhol | 1039.32 | kg/m3 | 298.20 | Optimization and modeling of extraction equilibria of the type 2 ternary systems containing (water + isovaleric acid + solvent) |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 432.00 ± 1.00 | K | 1.30 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.41951e+01 |
| Coeff. B | -4.57958e+03 |
| Coeff. C | -9.30050e+01 |
| Temperature range (K), min. | 422.29 |
| Temperature range (K), max. | 608.51 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | -4.76036e+01 |
| Coeff. B | -4.63994e+03 |
| Coeff. C | 9.97049e+00 |
| Coeff. D | -8.22302e-06 |

| | |
|---|---|
| Temperature range (K), min. | 275.15 |
| Temperature range (K), max. | 777.00 |

# Sources

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|---|---|
| **Phase equilibria for ternary liquid systems of (water + tetrahydrofuran + nonprotic aromatic solvent) at T = 298.2 K:** | https://www.doi.org/10.1016/j.jct.2005.07.010 |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Optimization and modeling of extraction equilibria of the type 2 ternary systems containing (water + isovaleric acid + solvent):** | https://www.doi.org/10.1016/j.jct.2015.07.035 |
| **KDB:** | https://www.cheric.org/files/research/kdb/mol/mol1032.mol |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C103504&Units=SI |
| **KDB Vapor Pressure Data:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1032 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Optimization of liquid-liquid equilibria of the type 2 ternary systems (water + valeric acid + aromatic solvent): Modeling through SERLAS:** | https://www.doi.org/10.1016/j.fluid.2016.01.050 |

# Legend

| | |
|---|---|
| **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 |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **nfpaf:** | NFPA Fire Rating |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **rhol:** | Liquid Density |
| **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 |