# 1,2-Benzenedicarboxylic acid

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|---|---|
| **Other names:** | 1,2-benzenedioic acid |
| | Acide phtalique |
| | Benzene-1,2-dicarboxylic acid |
| | Kyselina ftalova |
| | Orthophthalic acid |
| | Phthalic acid |
| | Sunftal 20 |
| | o-Benzenedicarboxylic acid |
| | o-Dicarboxybenzene |
| | o-Phthalic acid |
| | phenazopyridine |
| **Inchi:** | InChI=1S/C8H6O4/c9-7(10)5-3-1-2-4-6(5)8(11)12/h1-4H,(H,9,10)(H,11,12) |
| **InchiKey:** | XNGIFLGASWRNHJ-UHFFFAOYSA-N |
| **Formula:** | C8H6O4 |
| **SMILES:** | O=C(O)c1ccccc1C(=O)O |
| **Mol. weight [g/mol]:** | 166.13 |
| **CAS:** | 88-99-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -3223.50 ± 0.50 | kJ/mol | NIST Webbook |
| chs | -3223.70 | kJ/mol | NIST Webbook |
| chs | -3229.96 | kJ/mol | NIST Webbook |
| gf | -412.22 | kJ/mol | Joback Method |
| hf | -513.01 | kJ/mol | Joback Method |
| hfs | -781.91 | kJ/mol | NIST Webbook |
| hfs | -782.12 | kJ/mol | NIST Webbook |
| hfus | 21.50 | kJ/mol | Joback Method |
| hsub | 129.80 ± 0.60 | kJ/mol | NIST Webbook |
| hvap | 83.19 | kJ/mol | Joback Method |
| log10ws | -2.41 | | Aqueous Solubility Prediction Method |
| logp | 1.083 | | Crippen Method |
| mcvol | 114.700 | ml/mol | McGowan Method |
| pc | 5406.57 | kPa | Joback Method |
| rinpol | 1643.00 | | NIST Webbook |
| rinpol | 225.33 | | NIST Webbook |

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|---|---|---|---|
| ss | 207.94 | J/mol×K | NIST Webbook |
| tb | 706.20 | K | Joback Method |
| tc | 907.67 | K | Joback Method |
| tf | 480.00 ± 3.00 | K | NIST Webbook |
| vc | 0.425 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 289.37 | J/mol×K | 739.78 | Joback Method |
| cpg | 295.47 | J/mol×K | 773.36 | Joback Method |
| cpg | 282.80 | J/mol×K | 706.20 | Joback Method |
| cpg | 315.57 | J/mol×K | 907.67 | Joback Method |
| cpg | 311.15 | J/mol×K | 874.09 | Joback Method |
| cpg | 306.34 | J/mol×K | 840.51 | Joback Method |
| cpg | 301.12 | J/mol×K | 806.93 | Joback Method |
| cps | 201.70 | J/mol×K | 323.00 | NIST Webbook |
| cps | 201.70 | J/mol×K | 323.00 | NIST Webbook |
| cps | 188.11 | J/mol×K | 298.10 | NIST Webbook |
| dvisc | 0.0004918 | Pa×s | 484.67 | Joback Method |
| dvisc | 0.0000196 | Pa×s | 706.20 | Joback Method |
| dvisc | 0.0000314 | Pa×s | 661.89 | Joback Method |
| dvisc | 0.0000539 | Pa×s | 617.59 | Joback Method |
| dvisc | 0.0001006 | Pa×s | 573.28 | Joback Method |
| dvisc | 0.0002081 | Pa×s | 528.97 | Joback Method |
| dvisc | 0.0013822 | Pa×s | 440.36 | Joback Method |
| hfust | 36.50 | kJ/mol | 463.50 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 2.08639e+02 |
| Coeff. B | -2.17466e+04 |
| Coeff. C | -2.66695e+01 |
| Coeff. D | 7.96015e-06 |
| Temperature range (K), min. | 464.15 |

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|---|---|
| Temperature range (K), max. | 800.00 |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Solubilities of Phthalic Acid and o-Toluic Acid in Binary Acetic Acid + Water and Acetic Acid + o-Xylene Solvent Mixtures:** | https://www.doi.org/10.1021/acs.jced.6b00324 |
| **KDB Vapor Pressure Data:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=967 |
| **Solubility of o-Phthalic Acid in Methanol + Water and Methanol + Butyl Acetate from (298.15 to 333.15) K:** | https://www.doi.org/10.1021/je0600505 |
| **Solubilities of Benzenecarboxylic Acids in Isobutyl Acetate from (299.73 to 353.15) K:** | https://www.doi.org/10.1021/je101319f |
| **Solubility and Activity Coefficients of Acidic and Basic Nonelectrolytes in Aqueous Salt Solutions. 1. Solubility and Activity Coefficients of o-Phthalic Acid and L-Cystine in NaCl(aq), (CH3)4NCl(aq), and (C2H5)4NI(aq) at Different Ionic Strengths and at t ) 25 deg C:** | https://www.doi.org/10.1021/je0502039 |
| **Phase Equilibrium and Phase Diagram for the System of Benzene Dicarboxylic Acid + N-Methyl-2-pyrrolidone:** | https://www.doi.org/10.1021/je500542j |
| **KDB:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=967 |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Solubilities of Benzoic Acid and Phthalic Acid in Acetic Acid + Water Solvent Mixtures:** | https://www.doi.org/10.1021/je600527c |
| **Thermochemistry of Cs(hydrogen phthalate) and Cs2(terephthalate):** | https://www.doi.org/10.1016/j.tca.2005.01.024 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C88993&Units=SI |
| **Liquid-liquid equilibrium (LLE) data for ternary mixtures of [C4DMIM][PF6]+[PA]+[water] and [C4DMIM][PF6]+[PA]+[water] at T = 298.15 K and p = 1 atm:** | https://www.doi.org/10.1016/j.fluid.2014.08.004 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Solubility of mixed solids in supercritical carbon dioxide:** | https://www.doi.org/10.1016/j.fluid.2006.11.002 |
| **Solubilities of Terephthalic Acid, Phthalic Acid, and Isophthalic Acid in Tetrahydrofuran, Cyclohexanone, 1,2-Diethoxyethane, and Acetophenone:** | https://www.doi.org/10.1021/je9001976 |

# Legend

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|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **cps:** | Solid phase heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfs:** | Solid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hsub:** | Enthalpy of sublimation 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 |

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|---|---|
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |
| **ss:** | Solid phase molar entropy at standard conditions |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |