# Benzene, 1,3-dinitro-

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|---|---|
| **Other names:** | 1,3-Dinitrobenzene |
| | 1,3-Dinitrobenzol |
| | 2,4-Dinitrobenzene |
| | Benzene, m-dinitro- |
| | Dwunitrobenzen |
| | NSC 7189 |
| | m-Dinitrobenzene |
| | meta-Dinitrobenzene |
| **Inchi:** | InChI=1S/C6H4N2O4/c9-7(10)5-2-1-3-6(4-5)8(11)12/h1-4H |
| **InchiKey:** | WDCYWAQPCXBPJA-UHFFFAOYSA-N |
| **Formula:** | C6H4N2O4 |
| **SMILES:** | O=[N+]([O-])c1cccc([N+](=O)[O-])c1 |
| **Mol. weight [g/mol]:** | 168.11 |
| **CAS:** | 99-65-0 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -2908.00 | kJ/mol | NIST Webbook |
| chs | -2905.00 ± 0.40 | kJ/mol | NIST Webbook |
| chs | -2896.20 ± 2.90 | kJ/mol | NIST Webbook |
| chs | -2911.60 | kJ/mol | NIST Webbook |
| chs | -2913.49 | kJ/mol | NIST Webbook |
| chs | -2931.00 | kJ/mol | NIST Webbook |
| ea | 0.07 | eV | NIST Webbook |
| ea | 1.66 ± 0.10 | eV | NIST Webbook |
| ea | 1.65 ± 0.05 | eV | NIST Webbook |
| ea | 1.65 ± 0.05 | eV | NIST Webbook |
| gf | 173.52 | kJ/mol | Joback Method |
| hf | 36.37 | kJ/mol | Joback Method |
| hfl | -36.00 | kJ/mol | NIST Webbook |
| hfs | -19.20 | kJ/mol | NIST Webbook |
| hfs | -27.00 ± 0.40 | kJ/mol | NIST Webbook |
| hfus | 21.20 | kJ/mol | Phase Equilibria, Crystallization, and Microstructural Studies of Naphthalen-2-ol + 1,3-Dinitrobenzene |
| hsub | 87.00 ± 0.80 | kJ/mol | NIST Webbook |

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|---|---|---|---|
| hvap | 65.07 | kJ/mol | Joback Method |
| ie | 10.60 ± 0.10 | eV | NIST Webbook |
| ie | 10.40 | eV | NIST Webbook |
| ie | 10.43 ± 0.02 | eV | NIST Webbook |
| ie | 10.40 | eV | NIST Webbook |
| log10ws | -2.29 | | Estimated Solubility Method |
| log10ws | -2.29 | | Aqueous Solubility Prediction Method |
| logp | 1.503 | | Crippen Method |
| mcvol | 106.480 | ml/mol | McGowan Method |
| pc | 4730.11 | kPa | Joback Method |
| rinpol | 247.64 | | NIST Webbook |
| rinpol | 1400.00 | | NIST Webbook |
| rinpol | 247.45 | | NIST Webbook |
| rinpol | 247.64 | | NIST Webbook |
| rinpol | 248.35 | | NIST Webbook |
| tb | 570.20 | K | NIST Webbook |
| tc | 952.61 | K | Joback Method |
| tf | 363.00 ± 2.50 | K | NIST Webbook |
| tf | 363.00 ± 1.50 | K | NIST Webbook |
| tf | 363.23 ± 0.15 | K | NIST Webbook |
| tf | 362.65 ± 1.50 | K | NIST Webbook |
| tf | 362.40 ± 1.50 | K | NIST Webbook |
| tf | 362.40 | K | Aqueous Solubility Prediction Method |
| tf | 362.00 ± 2.00 | K | NIST Webbook |
| tf | 363.23 ± 0.20 | K | NIST Webbook |
| tf | 360.00 ± 0.10 | K | NIST Webbook |
| tf | 362.65 ± 0.30 | K | NIST Webbook |
| vc | 0.427 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 254.14 | J/mol×K | 672.02 | Joback Method |
| cpg | 263.06 | J/mol×K | 718.79 | Joback Method |
| cpg | 271.07 | J/mol×K | 765.55 | Joback Method |
| cpg | 278.24 | J/mol×K | 812.32 | Joback Method |
| cpg | 284.63 | J/mol×K | 859.08 | Joback Method |
| cpg | 290.30 | J/mol×K | 905.85 | Joback Method |
| cpg | 295.30 | J/mol×K | 952.61 | Joback Method |

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|---|---|---|---|---|
| cps | 197.50 | J/mol×K | 298.15 | NIST Webbook |
| cps | 180.30 | J/mol×K | 298.00 | NIST Webbook |
| cps | 188.30 | J/mol×K | 297.90 | NIST Webbook |
| hfust | 17.36 | kJ/mol | 363.20 | NIST Webbook |
| hfust | 17.36 | kJ/mol | 363.20 | NIST Webbook |
| hfust | 17.36 | kJ/mol | 363.20 | NIST Webbook |
| hfust | 17.35 | kJ/mol | 363.23 | NIST Webbook |
| hfust | 19.68 | kJ/mol | 360.40 | NIST Webbook |
| hsubt | 76.10 | kJ/mol | 345.50 | NIST Webbook |
| hsubt | 83.00 ± 2.00 | kJ/mol | 323.00 | NIST Webbook |
| hsubt | 81.10 ± 1.70 | kJ/mol | 322.00 | NIST Webbook |
| hvapt | 96.70 | kJ/mol | 357.50 | NIST Webbook |
| sfust | 47.80 | J/mol×K | 363.23 | NIST Webbook |
| sfust | 47.80 | J/mol×K | 363.20 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.57284e+01 |
| Coeff. B | -5.21731e+03 |
| Coeff. C | -1.00598e+02 |
| Temperature range (K), min. | 438.49 |
| Temperature range (K), max. | 601.45 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 1.26981e+02 |
| Coeff. B | -1.48701e+04 |
| Coeff. C | -1.54082e+01 |
| Coeff. D | 4.35894e-06 |
| Temperature range (K), min. | 364.00 |
| Temperature range (K), max. | 805.00 |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **KDB:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1438 |
| **KDB Vapor Pressure Data:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1438 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C99650&Units=SI |
| **Estimated Solubility Method:** | http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt |
| **A new semi-empirical model for correlating the solubilities of solids in supercritical carbon dioxide with cosolvents:** | https://www.doi.org/10.1016/j.fluid.2011.08.021 |
| **Phase Equilibria, Crystallization, and Microstructural Studies of Naphthalene-2-ol + 1,3- Dinitrobenzene:** | https://www.doi.org/10.1021/je100358e |
| **Solubilities of Benzene Derivatives in Supercritical Carbon Dioxide:** | https://www.doi.org/10.1021/je100863p |

# Legend

| | |
|---|---|
| **chl:** | Standard liquid enthalpy of combustion |
| **chs:** | Standard solid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **cps:** | Solid phase heat capacity |
| **ea:** | Electron affinity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfl:** | Liquid phase 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 |
| **hsubt:** | Enthalpy of sublimation at a given temperature |
| **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 |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |

| | |
|---|---|
| **sfust:** | Entropy of fusion at a given temperature |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |