# 1-Nitro-2-phenylethane

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|---|---|
| **Other names:** | (2-nitroethyl)benzene |
| | Benzene, (2-nitroethyl)- |
| **Inchi:** | InChI=1S/C8H9NO2/c10-9(11)7-6-8-4-2-1-3-5-8/h1-5H,6-7H2 |
| **InchiKey:** | XAWCLWKTUKMCMO-UHFFFAOYSA-N |
| **Formula:** | C8H9NO2 |
| **SMILES:** | O=[N+]([O-])CCc1ccccc1 |
| **Mol. weight [g/mol]:** | 151.16 |
| **CAS:** | 6125-24-2 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 164.44 | kJ/mol | Joback Method |
| hf | 17.32 | kJ/mol | Joback Method |
| hfus | 21.88 | kJ/mol | Joback Method |
| hvap | 52.27 | kJ/mol | Joback Method |
| log10ws | -2.36 | | Crippen Method |
| logp | 1.506 | | Crippen Method |
| mcvol | 117.240 | ml/mol | McGowan Method |
| pc | 3704.46 | kPa | Joback Method |
| rinpol | 1304.00 | | NIST Webbook |
| rinpol | 1262.00 | | NIST Webbook |
| rinpol | 1262.00 | | NIST Webbook |
| rinpol | 1255.00 | | NIST Webbook |
| rinpol | 1305.70 | | NIST Webbook |
| rinpol | 1300.00 | | NIST Webbook |
| rinpol | 1259.00 | | NIST Webbook |
| ripol | 2032.00 | | NIST Webbook |
| ripol | 2095.00 | | NIST Webbook |
| ripol | 2095.00 | | NIST Webbook |
| tb | 560.96 | K | Joback Method |
| tc | 804.48 | K | Joback Method |
| tf | 349.95 | K | Joback Method |
| vc | 0.458 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 266.02 | J/mol×K | 560.96 | Joback Method |
| cpg | 278.59 | J/mol×K | 601.55 | Joback Method |
| cpg | 290.21 | J/mol×K | 642.13 | Joback Method |
| cpg | 300.94 | J/mol×K | 682.72 | Joback Method |
| cpg | 310.82 | J/mol×K | 723.30 | Joback Method |
| cpg | 319.91 | J/mol×K | 763.89 | Joback Method |
| cpg | 328.26 | J/mol×K | 804.48 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.55677e+01 |
| Coeff. B | -4.70527e+03 |
| Coeff. C | -8.65860e+01 |
| Temperature range (K), min. | 394.52 |
| Temperature range (K), max. | 545.36 |

# Sources

| | |
|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C6125242&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 |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |

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