# Benzenemethanol, 2-nitro-

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|---|---|
| **Other names:** | Benzyl alcohol, o-nitro- |
| | o-Nitrobenzyl alcohol |
| | 2-Nitrobenzyl alcohol |
| **Inchi:** | InChI=1S/C7H7NO3/c9-5-6-3-1-2-4-7(6)8(10)11/h1-4,9H,5H2 |
| **InchiKey:** | BWRBVBFLFQKBPT-UHFFFAOYSA-N |
| **Formula:** | C7H7NO3 |
| **SMILES:** | O=[N+]([O-])c1ccccc1CO |
| **Mol. weight [g/mol]:** | 153.14 |
| **CAS:** | 612-25-9 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 9.57 | kJ/mol | Joback Method |
| hf | -125.74 | kJ/mol | Joback Method |
| hfus | 22.99 | kJ/mol | Joback Method |
| hvap | 67.38 | kJ/mol | Joback Method |
| log10ws | -2.27 | | Crippen Method |
| logp | 1.087 | | Crippen Method |
| mcvol | 109.020 | ml/mol | McGowan Method |
| pc | 4627.70 | kPa | Joback Method |
| tb | 543.20 | K | NIST Webbook |
| tc | 863.19 | K | Joback Method |
| tf | 412.02 | K | Joback Method |
| vc | 0.420 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 262.07 | J/mol×K | 635.24 | Joback Method |
| cpg | 270.91 | J/mol×K | 673.23 | Joback Method |
| cpg | 279.10 | J/mol×K | 711.22 | Joback Method |
| cpg | 286.68 | J/mol×K | 749.21 | Joback Method |
| cpg | 293.68 | J/mol×K | 787.21 | Joback Method |
| cpg | 300.14 | J/mol×K | 825.20 | Joback Method |

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|---|---|---|---|---|
| cpg | 306.09 | J/mol×K | 863.19 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 441.20 | K | 2.70 | NIST Webbook |

# Sources

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|---|---|
| **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=C612259&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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