# «alpha»-Nitroacetophenone

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|---|---|
| **Other names:** | Ethanone, 2-nitro-1-phenyl- |
| | Benzoylnitromethane |
| | Acetophenone, 2-nitro- |
| | «omega»-Nitroacetophenone |
| | 2-Nitro-1-phenylethanone |
| | 2-Nitroacetophenone |
| | Nitromethyl phenyl ketone |
| | NSC 4509 |
| **Inchi:** | InChI=1S/C8H7NO3/c10-8(6-9(11)12)7-4-2-1-3-5-7/h1-5H,6H2 |
| **InchiKey:** | JTWHVBNYYWFXSI-UHFFFAOYSA-N |
| **Formula:** | C8H7NO3 |
| **SMILES:** | O=C(C[N+](=O)[O-])c1ccccc1 |
| **Mol. weight [g/mol]:** | 165.15 |
| **CAS:** | 614-21-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 35.52 | kJ/mol | Joback Method |
| hf | -95.26 | kJ/mol | Joback Method |
| hfus | 23.48 | kJ/mol | Joback Method |
| hvap | 59.02 | kJ/mol | Joback Method |
| log10ws | -2.22 | | Crippen Method |
| logp | 1.146 | | Crippen Method |
| mcvol | 118.810 | ml/mol | McGowan Method |
| pc | 4005.77 | kPa | Joback Method |
| tb | 614.83 | K | Joback Method |
| tc | 865.79 | K | Joback Method |
| tf | 399.88 | K | Joback Method |
| vc | 0.464 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 277.61 | J/mol×K | 614.83 | Joback Method |

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|---|---|---|---|---|
| cpg | 288.62 | J/mol×K | 656.66 | Joback Method |
| cpg | 298.72 | J/mol×K | 698.48 | Joback Method |
| cpg | 307.93 | J/mol×K | 740.31 | Joback Method |
| cpg | 316.32 | J/mol×K | 782.14 | Joback Method |
| cpg | 323.95 | J/mol×K | 823.96 | Joback Method |
| cpg | 330.85 | J/mol×K | 865.79 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **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=C614211&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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