# (3-Nitrophenyl) methanol, ethyl ether

**Inchi:** InChI=1S/C9H11NO3/c1-2-13-7-8-4-3-5-9(6-8)10(11)12/h3-6H,2,7H2,1H3
**InchiKey:** VPUMBFVYZSOPAJ-UHFFFAOYSA-N
**Formula:** C9H11NO3
**SMILES:** CCOCc1cccc([N+](=O)[O-])c1
**Mol. weight [g/mol]:** 181.19

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 58.23 | kJ/mol | Joback Method |
| hf | -147.01 | kJ/mol | Joback Method |
| hfus | 25.27 | kJ/mol | Joback Method |
| hvap | 57.57 | kJ/mol | Joback Method |
| log10ws | -2.93 | | Crippen Method |
| logp | 2.131 | | Crippen Method |
| mcvol | 137.200 | ml/mol | McGowan Method |
| pc | 3188.33 | kPa | Joback Method |
| rinpol | 1509.00 | | NIST Webbook |
| rinpol | 1509.00 | | NIST Webbook |
| tb | 611.24 | K | Joback Method |
| tc | 847.17 | K | Joback Method |
| tf | 395.97 | K | Joback Method |
| vc | 0.531 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 334.13 | J/mol×K | 611.24 | Joback Method |
| cpg | 347.05 | J/mol×K | 650.56 | Joback Method |
| cpg | 359.12 | J/mol×K | 689.88 | Joback Method |
| cpg | 370.35 | J/mol×K | 729.20 | Joback Method |
| cpg | 380.77 | J/mol×K | 768.52 | Joback Method |
| cpg | 390.39 | J/mol×K | 807.85 | Joback Method |
| cpg | 399.25 | J/mol×K | 847.17 | Joback Method |

# 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=U374644&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |