# (3-Nitrophenyl) methanol, isopropyl ether

**Inchi:** InChI=1S/C10H13NO3/c1-8(2)14-7-9-4-3-5-10(6-9)11(12)13/h3-6,8H,7H2,1-2H3
**InchiKey:** JYLYIZFXTADDBT-UHFFFAOYSA-N
**Formula:** C10H13NO3
**SMILES:** CC(C)OCc1cccc([N+](=O)[O-])c1
**Mol. weight [g/mol]:** 195.22

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 64.21 | kJ/mol | Joback Method |
| hf | -172.93 | kJ/mol | Joback Method |
| hfus | 24.33 | kJ/mol | Joback Method |
| hvap | 59.41 | kJ/mol | Joback Method |
| log10ws | -3.46 | | Crippen Method |
| logp | 2.520 | | Crippen Method |
| mcvol | 151.290 | ml/mol | McGowan Method |
| pc | 2893.62 | kPa | Joback Method |
| rinpol | 1555.00 | | NIST Webbook |
| rinpol | 1555.00 | | NIST Webbook |
| tb | 633.68 | K | Joback Method |
| tc | 869.80 | K | Joback Method |
| tf | 392.24 | K | Joback Method |
| vc | 0.582 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 382.74 | J/mol×K | 633.68 | Joback Method |
| cpg | 396.77 | J/mol×K | 673.03 | Joback Method |
| cpg | 409.84 | J/mol×K | 712.39 | Joback Method |
| cpg | 421.98 | J/mol×K | 751.74 | Joback Method |
| cpg | 433.23 | J/mol×K | 791.09 | Joback Method |
| cpg | 443.60 | J/mol×K | 830.44 | Joback Method |
| cpg | 453.12 | J/mol×K | 869.80 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U374649&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# 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 |