# Propanamide, N-(3-nitrophenyl)-2-methyl-

**Inchi:** InChI=1S/C10H12N2O3/c1-7(2)10(13)11-8-4-3-5-9(6-8)12(14)15/h3-7H,1-2H3,(H,11,13)
**InchiKey:** YARNVNLKNTXUBT-UHFFFAOYSA-N
**Formula:** C10H12N2O3
**SMILES:** CC(C)C(=O)Nc1cccc([N+](=O)[O-])c1
**Mol. weight [g/mol]:** 208.21

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 129.68 | kJ/mol | Joback Method |
| hf | -99.82 | kJ/mol | Joback Method |
| hfus | 29.84 | kJ/mol | Joback Method |
| hvap | 70.18 | kJ/mol | Joback Method |
| log10ws | -2.92 | | Crippen Method |
| logp | 2.189 | | Crippen Method |
| mcvol | 156.970 | ml/mol | McGowan Method |
| pc | 3206.41 | kPa | Joback Method |
| rinpol | 1899.00 | | NIST Webbook |
| rinpol | 1899.00 | | NIST Webbook |
| tb | 715.30 | K | Joback Method |
| tc | 958.30 | K | Joback Method |
| tf | 472.60 | K | Joback Method |
| vc | 0.605 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 419.60 | J/mol×K | 715.30 | Joback Method |
| cpg | 431.83 | J/mol×K | 755.80 | Joback Method |
| cpg | 443.07 | J/mol×K | 796.30 | Joback Method |
| cpg | 453.37 | J/mol×K | 836.80 | Joback Method |
| cpg | 462.77 | J/mol×K | 877.30 | Joback Method |
| cpg | 471.34 | J/mol×K | 917.80 | Joback Method |
| cpg | 479.11 | J/mol×K | 958.30 | 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=U307325&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 |