# Benzamide, N-(3-methylphenyl)-4-nitro-

**Inchi:** InChI=1S/C14H12N2O3/c1-10-3-2-4-12(9-10)15-14(17)11-5-7-13(8-6-11)16(18)19/h2-9H
**InchiKey:** OJZGTNXZLKZWDC-UHFFFAOYSA-N
**Formula:** C14H12N2O3
**SMILES:** Cc1cccc(NC(=O)c2ccc([N+](=O)[O-])cc2)c1
**Mol. weight [g/mol]:** 256.26

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 268.58 | kJ/mol | Joback Method |
| hf | 47.96 | kJ/mol | Joback Method |
| hfus | 37.38 | kJ/mol | Joback Method |
| hvap | 82.41 | kJ/mol | Joback Method |
| log10ws | -4.57 | | Crippen Method |
| logp | 3.156 | | Crippen Method |
| mcvol | 189.570 | ml/mol | McGowan Method |
| pc | 2947.28 | kPa | Joback Method |
| rinpol | 2463.00 | | NIST Webbook |
| rinpol | 2463.00 | | NIST Webbook |
| tb | 838.92 | K | Joback Method |
| tc | 1101.14 | K | Joback Method |
| tf | 571.62 | K | Joback Method |
| vc | 0.727 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 533.12 | J/mol×K | 838.92 | Joback Method |
| cpg | 544.78 | J/mol×K | 882.62 | Joback Method |
| cpg | 555.28 | J/mol×K | 926.33 | Joback Method |
| cpg | 564.72 | J/mol×K | 970.03 | Joback Method |
| cpg | 573.17 | J/mol×K | 1013.74 | Joback Method |
| cpg | 580.72 | J/mol×K | 1057.44 | Joback Method |
| cpg | 587.48 | J/mol×K | 1101.14 | 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=U307351&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |