# Benzenamine, 3-nitro-N-phenyl-

**Other names:** Diphenylamine, 3-nitro-
m-Nitrodiphenylamine
3-Nitrodiphenylamine
**Inchi:** InChI=1S/C12H10N2O2/c15-14(16)12-8-4-7-11(9-12)13-10-5-2-1-3-6-10/h1-9,13H
**InchiKey:** VNRHTFXMONFRSL-UHFFFAOYSA-N
**Formula:** C12H10N2O2
**SMILES:** O=[N+]([O-])c1cccc(Nc2ccccc2)c1
**Mol. weight [g/mol]:** 214.22
**CAS:** 4531-79-7

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 390.29 | kJ/mol | Joback Method |
| hf | 213.29 | kJ/mol | Joback Method |
| hfus | 30.99 | kJ/mol | Joback Method |
| hvap | 70.55 | kJ/mol | Joback Method |
| log10ws | -3.93 | | Crippen Method |
| logp | 3.338 | | Crippen Method |
| mcvol | 159.820 | ml/mol | McGowan Method |
| pc | 3468.36 | kPa | Joback Method |
| tb | 734.31 | K | Joback Method |
| tc | 1004.26 | K | Joback Method |
| tf | 486.63 | K | Joback Method |
| vc | 0.609 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 421.30 | J/mol×K | 734.31 | Joback Method |
| cpg | 434.25 | J/mol×K | 779.30 | Joback Method |
| cpg | 445.95 | J/mol×K | 824.29 | Joback Method |
| cpg | 456.48 | J/mol×K | 869.29 | Joback Method |
| cpg | 465.95 | J/mol×K | 914.28 | Joback Method |
| cpg | 474.47 | J/mol×K | 959.27 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 482.14 | J/mol×K | 1004.26 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C4531797&Units=SI |

# 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 |