# N-(beta-dimethylaminoethyl)-o-phenylenediamine

**Inchi:** InChI=1S/C10H17N3/c1-13(2)8-7-12-10-6-4-3-5-9(10)11/h3-6,12H,7-8,11H2,1-2H3
**InchiKey:** YMYPZBOBAISUFL-UHFFFAOYSA-N
**Formula:** C10H17N3
**SMILES:** CN(C)CCNc1ccccc1N
**Mol. weight [g/mol]:** 179.26
**CAS:** 78156-03-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 402.72 | kJ/mol | Joback Method |
| hf | 130.12 | kJ/mol | Joback Method |
| hfus | 28.63 | kJ/mol | Joback Method |
| hvap | 59.91 | kJ/mol | Joback Method |
| log10ws | -0.94 | | Crippen Method |
| logp | 1.242 | | Crippen Method |
| mcvol | 157.940 | ml/mol | McGowan Method |
| pc | 3107.10 | kPa | Joback Method |
| tb | 595.00 | K | Joback Method |
| tc | 808.51 | K | Joback Method |
| tf | 409.79 | K | Joback Method |
| vc | 0.570 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 401.19 | J/mol×K | 595.00 | Joback Method |
| cpg | 416.19 | J/mol×K | 630.58 | Joback Method |
| cpg | 430.25 | J/mol×K | 666.17 | Joback Method |
| cpg | 443.41 | J/mol×K | 701.75 | Joback Method |
| cpg | 455.72 | J/mol×K | 737.34 | Joback Method |
| cpg | 467.22 | J/mol×K | 772.92 | Joback Method |
| cpg | 477.96 | J/mol×K | 808.51 | Joback Method |

# Sources

| | |
|---|---|
| **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=C78156033&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |