# Benzaldehyde, 4-(dimethylamino)-

| | |
|---|---|
| **Other names:** | Benzaldehyde, p-(dimethylamino)- |
| | p-(Dimethylamino)benzaldehyde |
| | p-(N,N-Dimethylamino)benzaldehyde |
| | p-Formyl-N,N-dimethylaniline |
| | p-Formyldimethylaniline |
| | Ehrlich's reagent |
| | 4-(Dimethylamino)benzaldehyde |
| | 4-Dimethylaminobenzenecarbonal |
| | para-Dimethylaminobenzaldehyde |
| | 4-N,N-Dimethylaminobenzaldehyde |
| | N,N-Dimethyl-p-aminobenzaldehyde |
| | Reagens ehrlichovo |
| | 4-Formyl-N,N-dimethylaniline |
| | N,N-Dimethyl-4-formylaniline |
| | N,N-Dimethyl-4-aminobenzaldehyde |
| | p-DAB |
| | NSC 5517 |
| **Inchi:** | InChI=1S/C9H11NO/c1-10(2)9-5-3-8(7-11)4-6-9/h3-7H,1-2H3 |
| **InchiKey:** | BGNGWHSBYQYVRX-UHFFFAOYSA-N |
| **Formula:** | C9H11NO |
| **SMILES:** | CN(C)c1ccc(C=O)cc1 |
| **Mol. weight [g/mol]:** | 149.19 |
| **CAS:** | 100-10-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 924.80 | kJ/mol | NIST Webbook |
| basg | 898.30 | kJ/mol | NIST Webbook |
| chs | -4977.00 | kJ/mol | NIST Webbook |
| chs | -4976.03 ± 0.84 | kJ/mol | NIST Webbook |
| gf | 138.94 | kJ/mol | Joback Method |
| hf | -22.08 | kJ/mol | Joback Method |
| hfs | -137.00 | kJ/mol | NIST Webbook |
| hfus | 18.03 | kJ/mol | Joback Method |
| hvap | 47.33 | kJ/mol | Joback Method |
| ie | 7.30 ± 0.10 | eV | NIST Webbook |
| ie | 7.81 | eV | NIST Webbook |

| | | | |
|---|---|---|---|
| ie | 7.36 ± 0.02 | eV | NIST Webbook |
| ie | 7.30 ± 0.10 | eV | NIST Webbook |
| log10ws | -1.62 | | Crippen Method |
| logp | 1.565 | | Crippen Method |
| mcvol | 125.460 | ml/mol | McGowan Method |
| pc | 3484.76 | kPa | Joback Method |
| rinpol | 1528.00 | | NIST Webbook |
| rinpol | 1481.00 | | NIST Webbook |
| rinpol | 1528.00 | | NIST Webbook |
| rinpol | 1528.00 | | NIST Webbook |
| rinpol | 1481.00 | | NIST Webbook |
| rinpol | 1528.00 | | NIST Webbook |
| ripol | 2459.00 | | NIST Webbook |
| ripol | 2459.00 | | NIST Webbook |
| tb | 498.08 | K | Joback Method |
| tc | 709.02 | K | Joback Method |
| tf | 347.00 | K | NIST Webbook |
| vc | 0.467 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 324.73 | J/mol×K | 673.86 | Joback Method |
| cpg | 267.08 | J/mol×K | 498.08 | Joback Method |
| cpg | 280.15 | J/mol×K | 533.24 | Joback Method |
| cpg | 292.41 | J/mol×K | 568.39 | Joback Method |
| cpg | 303.91 | J/mol×K | 603.55 | Joback Method |
| cpg | 314.67 | J/mol×K | 638.70 | Joback Method |
| cpg | 334.13 | J/mol×K | 709.02 | Joback Method |
| hfust | 19.07 | kJ/mol | 346.20 | NIST Webbook |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 449.70 | K | 2.30 | NIST Webbook |
| tbrp | 418.00 | K | 1.30 | NIST Webbook |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C100107&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

| | |
|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **chs:** | Standard solid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfs:** | Solid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |