# N-benzyl-n-methylamino-acetonitrile

**Inchi:** InChI=1S/C10H12N2/c1-12(8-7-11)9-10-5-3-2-4-6-10/h2-6H,8-9H2,1H3
**InchiKey:** KUSXDIGALTYDLG-UHFFFAOYSA-N
**Formula:** C10H12N2
**SMILES:** CN(CC#N)Cc1ccccc1
**Mol. weight [g/mol]:** 160.22
**CAS:** 14321-25-6

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 389.69 | kJ/mol | Joback Method |
| hf | 219.21 | kJ/mol | Joback Method |
| hfus | 20.22 | kJ/mol | Joback Method |
| hvap | 52.65 | kJ/mol | Joback Method |
| log10ws | -2.04 | | Crippen Method |
| logp | 1.642 | | Crippen Method |
| mcvol | 139.360 | ml/mol | McGowan Method |
| pc | 2847.48 | kPa | Joback Method |
| tb | 569.40 | K | Joback Method |
| tc | 789.25 | K | Joback Method |
| tf | 326.34 | K | Joback Method |
| vc | 0.531 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 322.93 | J/mol×K | 569.40 | Joback Method |
| cpg | 336.12 | J/mol×K | 606.04 | Joback Method |
| cpg | 348.41 | J/mol×K | 642.68 | Joback Method |
| cpg | 359.85 | J/mol×K | 679.32 | Joback Method |
| cpg | 370.50 | J/mol×K | 715.96 | Joback Method |
| cpg | 380.39 | J/mol×K | 752.60 | Joback Method |
| cpg | 389.58 | J/mol×K | 789.25 | Joback Method |

# Sources

| | |
|---|---|
| **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=C14321256&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |