# alpha.-Methylbenzylamine

| | |
|---|---|
| **Other names:** | Benzenemethanamine, «alpha»-methyl-, (.+/-.)- |
| | Benzylamine, «alpha»-methyl-, (.+/-.)- |
| | (.+/-.)-«alpha»-Methylbenzylamine |
| | (.+/-.)-«alpha»-Phenylethylamine |
| | (.+/-.)-1-Phenethylamine |
| | (.+/-.)-1-Phenylethylamine |
| | DL-«alpha»-Phenylethylamine |
| | DL-1-Phenylethylamine |
| | Benzenemethanamine, «alpha»-methyl-, (±)- |
| | Benzylamine, «alpha»-methyl-, (±)- |
| | 1-Amino-1-phenylethane |
| | 1-Phenylethylamine |
| | Benzenemethanamine, «alpha»-methyl- |
| | DL-«alpha»-Methylbenzylamine |
| | Ethanamine, 1-phenyl- |
| | NSC 8391 |
| | «alpha»-methyl benzylamine |
| **Inchi:** | InChI=1S/C8H11N/c1-7(9)8-5-3-2-4-6-8/h2-7H,9H2,1H3 |
| **InchiKey:** | RQEUFEKYXDPUSK-UHFFFAOYSA-N |
| **Formula:** | C8H11N |
| **SMILES:** | CC(N)c1ccccc1 |
| **Mol. weight [g/mol]:** | 121.18 |
| **CAS:** | 98-84-0 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 192.90 | kJ/mol | Joback Method |
| hf | 56.59 | kJ/mol | Joback Method |
| hfus | 12.19 | kJ/mol | Joback Method |
| hvap | 54.90 ± 0.30 | kJ/mol | NIST Webbook |
| log10ws | -2.17 | | Crippen Method |
| logp | 1.706 | | Crippen Method |
| mcvol | 109.800 | ml/mol | McGowan Method |
| pc | 3955.54 | kPa | Joback Method |
| rinpol | 1050.00 | | NIST Webbook |
| rinpol | 1029.00 | | NIST Webbook |
| rinpol | 1019.50 | | NIST Webbook |

| | | | |
|---|---|---|---|
| rinpol | 1029.00 | | NIST Webbook |
| rinpol | 1031.00 | | NIST Webbook |
| rinpol | 1031.00 | | NIST Webbook |
| tb | 481.21 | K | Joback Method |
| tc | 709.62 | K | Joback Method |
| tf | 274.60 | K | Joback Method |
| vc | 0.399 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 228.83 | J/mol×K | 481.21 | Joback Method |
| cpg | 242.28 | J/mol×K | 519.28 | Joback Method |
| cpg | 254.86 | J/mol×K | 557.35 | Joback Method |
| cpg | 266.60 | J/mol×K | 595.41 | Joback Method |
| cpg | 277.54 | J/mol×K | 633.48 | Joback Method |
| cpg | 287.73 | J/mol×K | 671.55 | Joback Method |
| cpg | 297.20 | J/mol×K | 709.62 | Joback Method |
| hvapt | 54.70 ± 0.30 | kJ/mol | 300.50 | NIST Webbook |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C98840&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
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

# 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

| | |
|---|---|
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **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 |