# Benzenemethanamine, N-phenyl-

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|---|---|
| **Other names:** | Benzylamine, N-phenyl- |
| | Aniline, N-benzyl- |
| | Benzenamine, N-(phenylmethyl)- |
| | Benzylaniline |
| | Benzylphenylamine |
| | N-Benzylaniline |
| | N-Monobenzylaniline |
| | N-Phenylbenzylamine |
| | Phenylbenzylamine |
| | N-Phenylbenzenemethanamine |
| | NSC 147284 |
| **Inchi:** | InChI=1S/C13H13N/c1-3-7-12(8-4-1)11-14-13-9-5-2-6-10-13/h1-10,14H,11H2 |
| **InchiKey:** | GTWJETSWSUWSEJ-UHFFFAOYSA-N |
| **Formula:** | C13H13N |
| **SMILES:** | c1ccc(CNc2ccccc2)cc1 |
| **Mol. weight [g/mol]:** | 183.25 |
| **CAS:** | 103-32-2 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 372.79 | kJ/mol | Joback Method |
| hf | 214.88 | kJ/mol | Joback Method |
| hfus | 22.61 | kJ/mol | Joback Method |
| hvap | 55.52 | kJ/mol | Joback Method |
| log10ws | -3.59 | | Crippen Method |
| logp | 3.299 | | Crippen Method |
| mcvol | 156.490 | ml/mol | McGowan Method |
| pc | 3117.52 | kPa | Joback Method |
| tb | 579.70 | K | NIST Webbook |
| tb | 579.50 ± 0.50 | K | NIST Webbook |
| tc | 843.03 | K | Joback Method |
| tf | 311.00 ± 1.00 | K | NIST Webbook |
| tf | 305.15 ± 0.50 | K | NIST Webbook |
| tf | 310.00 ± 1.00 | K | NIST Webbook |
| vc | 0.583 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 433.32 | J/mol×K | 762.15 | Joback Method |
| cpg | 445.08 | J/mol×K | 802.59 | Joback Method |
| cpg | 374.82 | J/mol×K | 600.37 | Joback Method |
| cpg | 391.33 | J/mol×K | 640.81 | Joback Method |
| cpg | 406.53 | J/mol×K | 681.26 | Joback Method |
| cpg | 420.50 | J/mol×K | 721.70 | Joback Method |
| cpg | 455.85 | J/mol×K | 843.03 | Joback Method |
| hfust | 16.76 | kJ/mol | 305.60 | NIST Webbook |
| hfust | 16.76 | kJ/mol | 305.60 | NIST Webbook |
| hsubt | 103.60 ± 1.60 | kJ/mol | 302.50 | NIST Webbook |
| hvapt | 79.60 ± 1.10 | kJ/mol | 329.50 | NIST Webbook |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 475.20 | K | 4.90 | NIST Webbook |
| tbrp | 475.00 ± 1.00 | K | 4.90 | NIST Webbook |

# 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=C103322&Units=SI

# Legend

**cpg:** Ideal gas heat capacity
**gf:** Standard Gibbs free energy of formation

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|---|---|
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hsubt:** | Enthalpy of sublimation at a given temperature |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |