Benzenemethanamine, N-methyl-

Other names: Benzeneamine, N-methyl

Benzylamine, N-methyl-Benzylmethylamine

Methylbenzylamine

N-Benzyl-N-methylamine N-Benzylmethylamine N-Methy-N-benzylamine

N-Methyl(phenyl)methanamine N-Methyl-N-(phenylmethyl)amine N-methyl-1-phenylmethanamine

N-methylbenzylamine

NSC 8059

InChl=1S/C8H11N/c1-9-7-8-5-3-2-4-6-8/h2-6,9H,7H2,1H3

InchiKey: RIWRFSMVIUAEBX-UHFFFAOYSA-N

Formula: C8H11N

SMILES: CNCc1ccccc1

Mol. weight [g/mol]: 121.18 CAS: 103-67-3

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| gf | 218.28 | kJ/mol | Joback Method |
| hf | 81.55 | kJ/mol | Joback Method |
| hfus | 15.62 | kJ/mol | Joback Method |
| hvap | 42.11 | kJ/mol | Joback Method |
| ie | 8.65 | eV | NIST Webbook |
| ie | 8.73 | eV | NIST Webbook |
| log10ws | -1.96 | | Crippen Method |
| logp | 1.406 | | Crippen Method |
| mcvol | 109.800 | ml/mol | McGowan Method |
| рс | 3708.97 | kPa | Joback Method |
| rinpol | 1026.00 | | NIST Webbook |
| rinpol | 1078.00 | | NIST Webbook |
| rinpol | 1026.00 | | NIST Webbook |
| tb | 459.70 | K | NIST Webbook |
| tb | 453.70 | K | NIST Webbook |
| tc | 671.67 | K | Joback Method |

| tf | 259.00 | K | Joback Method |
|----|--------|---------|---------------|
| VC | 0.410 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---|
| cpg | 286.49 | J/mol×K | 671.67 | Joback Method |
| cpg | 276.83 | J/mol×K | 636.28 | Joback Method |
| cpg | 266.53 | J/mol×K | 600.88 | Joback Method |
| cpg | 255.53 | J/mol×K | 565.48 | Joback Method |
| cpg | 243.81 | J/mol×K | 530.08 | Joback Method |
| cpg | 231.34 | J/mol×K | 494.69 | Joback Method |
| cpg | 218.08 | J/mol×K | 459.29 | Joback Method |
| rhol | 851.00 | kg/m3 | 398.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines |
| rhol | 917.60 | kg/m3 | 323.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines |
| rhol | 913.30 | kg/m3 | 328.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines |
| rhol | 908.90 | kg/m3 | 333.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines |

| rhol | 904.50 | kg/m3 | 338.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
|------|--------|-------|--------|---|--|
| rhol | 900.00 | kg/m3 | 343.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 895.60 | kg/m3 | 348.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 891.20 | kg/m3 | 353.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 886.70 | kg/m3 | 358.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 882.30 | kg/m3 | 363.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 877.80 | kg/m3 | 368.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |

| rhol | 873.40 | kg/m3 | 373.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
|------|--------|-------|--------|---|--|
| rhol | 868.90 | kg/m3 | 378.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 864.40 | kg/m3 | 383.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 860.00 | kg/m3 | 388.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 855.40 | kg/m3 | 393.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 922.00 | kg/m3 | 318.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 846.40 | kg/m3 | 403.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |

| rhol | 841.80 | kg/m3 | 408.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
|------|--------|-------|--------|---|--|
| rhol | 837.30 | kg/m3 | 413.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 832.60 | kg/m3 | 418.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 944.55 | kg/m3 | 293.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 940.23 | kg/m3 | 298.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 935.90 | kg/m3 | 303.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 931.57 | kg/m3 | 308.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |

| rhol | 927.24 | kg/m3 | 313.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
|------|--------|-------|--------|---|--|
| rhol | 922.90 | kg/m3 | 318.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 918.55 | kg/m3 | 323.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 914.19 | kg/m3 | 328.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 909.83 | kg/m3 | 333.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 905.50 | kg/m3 | 338.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 901.19 | kg/m3 | 343.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |

| rhol | 926.40 | kg/m3 | 313.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
|------|--------|-------|--------|---|--|
| rhol | 930.70 | kg/m3 | 308.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 935.10 | kg/m3 | 303.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 939.60 | kg/m3 | 298.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 944.00 | kg/m3 | 293.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 948.40 | kg/m3 | 288.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |
| rhol | 952.80 | kg/m3 | 283.15 | Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines | |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 351.20 | K | 1.90 | NIST Webbook |

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C103673&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

https://www.doi.org/10.1021/acs.jced.6b00667 https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity

gf: Standard Gibbs free energy of formationhf: Enthalpy of formation at standard conditionshfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

ie: Ionization energy

log10ws:Log10 of Water solubility in mol/llogp:Octanol/Water partition coefficientmcvol:McGowan's characteristic volume

pc: Critical Pressurerhol: Liquid Density

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperaturetbrp: Boiling point at reduced pressure

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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