# Benzenemethanamine, «alpha»-methyl-, (R)-

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|---|---|
| **Other names:** | (R)-«alpha»-Methylbenzenemethanamine |
| | (S)-(-)-.alpha.methylbenzylamine |
| | (S)-(-)-1-phenylethylamine |
| | D-«alpha»-methylbenzylamine |
| | benzylamine, (S)-(-)-.alpha.-methyl- |
| **Inchi:** | InChI=1S/C8H11N/c1-7(9)8-5-3-2-4-6-8/h2-7H,9H2,1H3/t7-/m0/s1 |
| **InchiKey:** | RQEUFEKYXDPUSK-ZETCQYMHSA-N |
| **Formula:** | C8H11N |
| **SMILES:** | CC(N)c1ccccc1 |
| **Mol. weight [g/mol]:** | 121.18 |
| **CAS:** | 3886-69-9 |

## 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 | 54.10 ± 0.10 | 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 |
| tb | 460.20 | K | NIST Webbook |
| 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 | 287.73 | J/mol×K | 671.55 | Joback Method |
| 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 |

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|---|---|---|---|---|
| cpg | 266.60 | J/mol×K | 595.41 | Joback Method |
| cpg | 277.54 | J/mol×K | 633.48 | Joback Method |
| cpg | 297.20 | J/mol×K | 709.62 | Joback Method |
| rhol | 965.49 | kg/m3 | 298.15 | Enthalpic changes on mixing two couples of S- and R-enantiomers of benzyl-(1-phenyl-ethyl)-amine, 1-phenylethylamine, 1-phenyl-ethanol, butyric acid oxiranylmethyl ester, 4-methyl-[1,3]dioxolan-2-one, 2-chloro-methyloxirane and 3-hydroxyisobutyric acid methyl ester at T = 298.15 K |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 453.70 | K | 102.00 | NIST Webbook |

# Sources

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|---|---|
| **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=C3886699&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Enthalpic changes on mixing two couples of S- and R-enantiomers of benzyl-(1-phenyl-ethyl)-amine, 1-phenylethylamine, 1-phenyl-ethanol, butyric acid oxiranylmethyl ester, 4-methyl-[1,3]dioxolan-2-one, 2-chloro-methyloxirane and 3-hydroxyisobutyric acid methyl ester at T = 298.15 K:** | https://www.doi.org/10.1016/j.jct.2005.10.019 |

# 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 |

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|---|---|
| **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 |
| **rhol:** | Liquid Density |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |