

2,5-Dimethylbenzylamine

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| Inchi: | InChI=1S/C9H13N/c1-7-3-4-8(2)9(5-7)6-10/h3-5H,6,10H2,1-2H3 |
| InchiKey: | LUJNPFWZXIGIPS-UHFFFAOYSA-N |
| Formula: | C9H13N |
| SMILES: | <chem>Cc1ccc(C)c(CN)c1</chem> |
| Mol. weight [g/mol]: | 135.21 |
| CAS: | 93-48-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 184.50 | kJ/mol | Joback Method |
| hf | 18.29 | kJ/mol | Joback Method |
| hfus | 17.53 | kJ/mol | Joback Method |
| hvap | 49.87 | kJ/mol | Joback Method |
| log10ws | -2.74 | | Crippen Method |
| logp | 1.762 | | Crippen Method |
| mcvol | 123.890 | ml/mol | McGowan Method |
| pc | 3364.54 | kPa | Joback Method |
| rinpol | 1200.00 | | NIST Webbook |
| rinpol | 1200.00 | | NIST Webbook |
| tb | 514.49 | K | Joback Method |
| tc | 736.31 | K | Joback Method |
| tf | 325.91 | K | Joback Method |
| vc | 0.461 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 271.48 | J/molxK | 514.49 | Joback Method |
| cpg | 284.80 | J/molxK | 551.46 | Joback Method |
| cpg | 297.37 | J/molxK | 588.43 | Joback Method |
| cpg | 309.24 | J/molxK | 625.40 | Joback Method |
| cpg | 320.42 | J/molxK | 662.37 | Joback Method |
| cpg | 330.93 | J/molxK | 699.34 | Joback Method |
| cpg | 340.81 | J/molxK | 736.31 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C93481&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

Legend

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|------------------|---|
| 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 |
| h vap: | 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 |
| r in pol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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