

# Benzenemethanamine, N-ethyl-N-phenyl-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Benzylamine, N-ethyl-N-phenyl-<br>Benzylethylphenylamine<br>Ethylbenzylaniline<br>N-Benzyl-N-ethylaniline<br>N-Ethyl-N-benzylaniline<br>N-Ethyl-N-phenylbenzylamine<br>N,N-Benzylethylaniline<br>Phenylethylbenzylamine<br>UN 2274<br>NSC 1805 |
| <b>Inchi:</b>               | InChI=1S/C15H17N/c1-2-16(15-11-7-4-8-12-15)13-14-9-5-3-6-10-14/h3-12H,2,13H2,1H3   |
| <b>InchiKey:</b>            | HSZCJVZRHXPICIA-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C15H17N  |
| <b>SMILES:</b>              | CCN(Cc1ccccc1)c1ccccc1   |
| <b>Mol. weight [g/mol]:</b> | 211.30   |
| <b>CAS:</b>                 | 92-59-1  |

## Physical Properties

| Property code | Value         | Unit    | Source         |
|---------------|---------------|---------|----------------|
| gf            | 411.02        | kJ/mol  | Joback Method  |
| hf            | 187.66        | kJ/mol  | Joback Method  |
| hfus          | 25.71         | kJ/mol  | Joback Method  |
| hvap          | 55.58         | kJ/mol  | Joback Method  |
| log10ws       | -3.91         |         | Crippen Method |
| logp          | 3.713         |         | Crippen Method |
| mcvol         | 184.670       | ml/mol  | McGowan Method |
| pc            | 2505.01       | kPa     | Joback Method  |
| rinpol        | 1727.80       |         | NIST Webbook   |
| rinpol        | 1727.80       |         | NIST Webbook   |
| tb            | 608.40        | K       | Joback Method  |
| tc            | 839.25        | K       | Joback Method  |
| tf            | 308.00 ± 1.00 | K       | NIST Webbook   |
| vc            | 0.677         | m3/kmol | Joback Method  |

# Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 459.00 | J/mol×K | 608.40          | Joback Method |
| cpg           | 477.58 | J/mol×K | 646.87          | Joback Method |
| cpg           | 494.77 | J/mol×K | 685.35          | Joback Method |
| cpg           | 510.66 | J/mol×K | 723.82          | Joback Method |
| cpg           | 525.33 | J/mol×K | 762.30          | Joback Method |
| cpg           | 538.86 | J/mol×K | 800.77          | Joback Method |
| cpg           | 551.35 | J/mol×K | 839.25          | Joback Method |

# Pressure Dependent Properties

| Property code | Value         | Unit | Pressure [kPa] | Source       |
|---------------|---------------|------|----------------|--------------|
| tbrp          | 436.70        | K    | 0.80           | NIST Webbook |
| tbrp          | 458.70        | K    | 2.90           | NIST Webbook |
| tbrp          | 459.10 ± 0.50 | K    | 2.90           | NIST Webbook |

## Sources

|                 |   |
|-----------------|---|
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                   |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                   |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C92591&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C92591&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                               |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                       |

## Legend

|              |   |
|--------------|---|
| <b>cpg:</b>  | Ideal gas heat capacity                         |
| <b>gf:</b>   | Standard Gibbs free energy of formation         |
| <b>hf:</b>   | Enthalpy of formation at standard conditions    |
| <b>hfus:</b> | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b> | Enthalpy of vaporization at standard conditions |

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>mcvol:</b>   | McGowan's characteristic volume     |
| <b>pc:</b>      | Critical Pressure                   |
| <b>rinpol:</b>  | Non-polar retention indices         |
| <b>tb:</b>      | Normal Boiling Point Temperature    |
| <b>tbrp:</b>    | Boiling point at reduced pressure   |
| <b>tc:</b>      | Critical Temperature                |
| <b>tf:</b>      | Normal melting (fusion) point       |
| <b>vc:</b>      | Critical Volume                     |

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