

# Benzenemethanamine, N-phenyl-N-(phenylmethyl)-

Other names:

Aniline, N,N-dibenzyl-  
Benzenamine, N,N-bis(phenylmethyl)-  
Dibenzylamine, N-phenyl-  
Dibenzylaniline  
Dibenzylaniline, N,N-bis(phenylmethyl)-  
N-Phenyldibenzylamine  
N,N-Dibenzylaniline  
Aniline, N,N-bis(benzyl)-  
NSC 6243  
Aniline, dibenzyl-

**Inchi:** InChI=1S/C20H19N/c1-4-10-18(11-5-1)16-21(20-14-8-3-9-15-20)17-19-12-6-2-7-13-19/h

**InchiKey:** ISGXOWLMGOPVPB-UHFFFAOYSA-N

**Formula:** C20H19N

**SMILES:** c1ccc(CN(Cc2ccccc2)c2ccccc2)cc1

**Mol. weight [g/mol]:** 273.37

**CAS:** 91-73-6

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 565.53  | kJ/mol  | Joback Method  |
| hf            | 320.99  | kJ/mol  | Joback Method  |
| hfus          | 32.70   | kJ/mol  | Joback Method  |
| hvap          | 68.98   | kJ/mol  | Joback Method  |
| log10ws       | -5.60   |         | Crippen Method |
| logp          | 4.893   |         | Crippen Method |
| mcvol         | 231.360 | ml/mol  | McGowan Method |
| pc            | 2169.38 | kPa     | Joback Method  |
| tb            | 749.48  | K       | Joback Method  |
| tc            | 1001.69 | K       | Joback Method  |
| tf            | 426.89  | K       | Joback Method  |
| vc            | 0.850   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 644.45 | J/mol×K | 749.48          | Joback Method |
| cpg           | 662.95 | J/mol×K | 791.52          | Joback Method |
| cpg           | 679.83 | J/mol×K | 833.55          | Joback Method |
| cpg           | 695.22 | J/mol×K | 875.59          | Joback Method |
| cpg           | 709.29 | J/mol×K | 917.62          | Joback Method |
| cpg           | 722.19 | J/mol×K | 959.66          | Joback Method |
| cpg           | 734.06 | J/mol×K | 1001.69         | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                   |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                   |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C91736&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C91736&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                               |
| <b>Crippen Method:</b> | <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>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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