

# Benzenemethanamine, N,N-diphenyl-

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Other names:         | Benzenemethanamine, N,N-diphenyl-                                                 |
| Inchi:               | InChI=1S/C19H17N/c1-4-10-17(11-5-1)16-20(18-12-6-2-7-13-18)19-14-8-3-9-15-19/h1-1 |
| InchiKey:            | FKJARBPQBIATJT-UHFFFAOYSA-N                                                       |
| Formula:             | C19H17N                                                                           |
| SMILES:              | c1ccc(CN(c2ccccc2)c2ccccc2)cc1                                                    |
| Mol. weight [g/mol]: | 259.35                                                                            |

## Physical Properties

| Property code | Value             | Unit    | Source             |
|---------------|-------------------|---------|--------------------|
| af            | 0.5830            |         | Cheméo Relay (1.0) |
| chs           | -10091.00 ± 10.00 | kJ/mol  | NIST Webbook       |
| hf            | 326.46            | kJ/mol  | Cheméo Relay (1.0) |
| hfs           | 185.00 ± 10.00    | kJ/mol  | NIST Webbook       |
| hfus          | 30.11             | kJ/mol  | Joback Method      |
| hvap          | 92.53             | kJ/mol  | Cheméo Relay (1.0) |
| ie            | 7.41              | eV      | Cheméo Relay (1.0) |
| log10ws       | -5.44             |         | Cheméo Relay (1.0) |
| logp          | 5.025             |         | Crippen Method     |
| mcvol         | 217.270           | ml/mol  | McGowan Method     |
| pc            | 2377.22           | kPa     | Joback Method      |
| tb            | 645.07            | K       | Cheméo Relay (1.0) |
| tc            | 958.27            | K       | Cheméo Relay (1.0) |
| tf            | 330.05            | K       | Cheméo Relay (1.0) |
| vc            | 0.786             | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 589.67 | J/mol×K | 726.60          | Joback Method |
| cpg           | 608.11 | J/mol×K | 769.60          | Joback Method |
| cpg           | 624.86 | J/mol×K | 812.60          | Joback Method |
| cpg           | 640.08 | J/mol×K | 855.60          | Joback Method |
| cpg           | 653.92 | J/mol×K | 898.61          | Joback Method |
| cpg           | 666.54 | J/mol×K | 941.61          | Joback Method |

## Sources

|                           |                                                                                                                                           |
|---------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method:           | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| Cheméo Relay (1.0):       |                                                                                                                                           |
| Cheméo Relay (1.0, beta): |                                                                                                                                           |
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C606871&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C606871&amp;Units=SI</a> |
| 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>                     |
| Crippen Method:           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |

## Legend

|                 |                                                          |
|-----------------|----------------------------------------------------------|
| <b>af:</b>      | Acentric Factor                                          |
| <b>chs:</b>     | Standard solid enthalpy of combustion                    |
| <b>cpg:</b>     | Ideal gas heat capacity                                  |
| <b>hf:</b>      | Enthalpy of formation at standard conditions             |
| <b>hfs:</b>     | Solid phase 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>ie:</b>      | Ionization energy                                        |
| <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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