

# 4,4'-BENZYLIDENE BIS(N,N-DIMETHYLANILINE)

|                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
|----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | Leuco malachite green<br>Benzenamine, 4,4'-(phenylmethylene)bis[N,N-dimethyl-<br>Aniline, 4,4'-benzylidenebis(N,N-dimethyl-<br>Bis(p-dimethylaminophenyl)phenylmethane<br>Bis(p-(N,N-dimethylamino)phenyl)phenylmethane<br>Bis(4,4'-(dimethylamino)phenyl)phenyl methane<br>C.I. Basic Green 4, leuco base<br>Malachite green leuco<br>Malachite green leuco base<br>Tetramethyldiaminotriphenylmethane<br>4,4'-Benzylidene bis(N,N-dimethylaniline)<br>4,4'-Bis(dimethylamino)triphenylmethane<br>4,4'-Bis(N,N-dimethylaminophenyl)phenylmethane<br>NSC 36379<br>N,N,N',N'-tetramethyl-4,4'-benzylidenedianiline |
| Inchi:               | InChI=1S/C23H26N2/c1-24(2)21-14-10-19(11-15-21)23(18-8-6-5-7-9-18)20-12-16-22(17-13-23)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| InchiKey:            | WZKXBGJNNCGHIC-UHFFFAOYSA-N                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| Formula:             | C23H26N2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| SMILES:              | CN(C)c1ccc(C(c2ccccc2)c2ccc(N(C)C)cc2)cc1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| Mol. weight [g/mol]: | 330.47                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |

## Physical Properties

| Property code | Value   | Unit    | Source             |
|---------------|---------|---------|--------------------|
| af            | 0.7106  |         | Cheméo Relay (1.0) |
| gf            | 679.87  | kJ/mol  | Joback Method      |
| hf            | 273.37  | kJ/mol  | Cheméo Relay (1.0) |
| hfus          | 39.19   | kJ/mol  | Joback Method      |
| hvap          | 109.35  | kJ/mol  | Cheméo Relay (1.0) |
| ie            | 6.94    | eV      | Cheméo Relay (1.0) |
| log10ws       | -6.33   |         | Cheméo Relay (1.0) |
| logp          | 4.999   |         | Crippen Method     |
| mcvol         | 283.610 | ml/mol  | McGowan Method     |
| pc            | 1653.80 | kPa     | Joback Method      |
| tb            | 701.43  | K       | Cheméo Relay (1.0) |
| tc            | 1000.19 | K       | Cheméo Relay (1.0) |
| tf            | 424.02  | K       | Cheméo Relay (1.0) |
| vc            | 1.018   | m3/kmol | Cheméo Relay (1.0) |

# Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 855.62 | J/mol×K | 840.08          | Joback Method |
| cpg           | 873.99 | J/mol×K | 880.11          | Joback Method |
| cpg           | 890.91 | J/mol×K | 920.13          | Joback Method |
| cpg           | 906.51 | J/mol×K | 960.16          | Joback Method |
| cpg           | 920.92 | J/mol×K | 1000.18         | Joback Method |
| cpg           | 934.30 | J/mol×K | 1040.21         | Joback Method |
| cpg           | 946.78 | J/mol×K | 1080.24         | Joback Method |

## Sources

|                           |                                                                                                                                           |
|---------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| 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>                                 |
| Crippen Method:           | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=C129737&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C129737&amp;Units=SI</a> |
| Joback Method:            | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |

## Legend

|          |                                                 |
|----------|-------------------------------------------------|
| af:      | Acentric Factor                                 |
| 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       |
| hvap:    | Enthalpy of vaporization at standard conditions |
| ie:      | Ionization energy                               |
| log10ws: | Log10 of Water solubility in mol/l              |
| logp:    | Octanol/Water partition coefficient             |
| mcvol:   | McGowan's characteristic volume                 |
| pc:      | 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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