

# Naphthalene, 2,6-bis(1,1-dimethylethyl)-

|                             |                                                                                  |
|-----------------------------|----------------------------------------------------------------------------------|
| <b>Other names:</b>         | Naphthalene, 2,6-di-tert-butyl-<br>2,6-Di-tert-butyl-naphthalene                 |
| <b>Inchi:</b>               | InChI=1S/C18H24/c1-17(2,3)15-9-7-14-12-16(18(4,5)6)10-8-13(14)11-15/h7-12H,1-6H3 |
| <b>InchiKey:</b>            | TZGXZNWUOXLMFL-UHFFFAOYSA-N                                                      |
| <b>Formula:</b>             | C18H24                                                                           |
| <b>SMILES:</b>              | CC(C)(C)c1ccc2cc(C(C)(C)C)ccc2c1                                                 |
| <b>Mol. weight [g/mol]:</b> | 240.38                                                                           |
| <b>CAS:</b>                 | 3905-64-4                                                                        |

## Physical Properties

| Property code | Value          | Unit                 | Source         |
|---------------|----------------|----------------------|----------------|
| gf            | 306.16         | kJ/mol               | Joback Method  |
| hf            | -27.69         | kJ/mol               | Joback Method  |
| hfus          | 17.83          | kJ/mol               | Joback Method  |
| hvap          | 58.31          | kJ/mol               | Joback Method  |
| log10ws       | -5.90          |                      | Crippen Method |
| logp          | 5.435          |                      | Crippen Method |
| mvol          | 221.260        | ml/mol               | McGowan Method |
| pc            | 1792.42        | kPa                  | Joback Method  |
| tb            | 603.00 ± 25.00 | K                    | NIST Webbook   |
| tc            | 893.08         | K                    | Joback Method  |
| tf            | 419.00 ± 4.00  | K                    | NIST Webbook   |
| vc            | 0.836          | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 600.68 | J/mol×K | 660.40          | Joback Method |
| cpg           | 620.51 | J/mol×K | 699.18          | Joback Method |
| cpg           | 638.89 | J/mol×K | 737.96          | Joback Method |
| cpg           | 655.94 | J/mol×K | 776.74          | Joback Method |
| cpg           | 671.81 | J/mol×K | 815.52          | Joback Method |
| cpg           | 686.64 | J/mol×K | 854.30          | Joback Method |
| cpg           | 700.58 | J/mol×K | 893.08          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0016138 | Paxs | 381.62 | Joback Method |
| dvisc | 0.0008831 | Paxs | 428.08 | Joback Method |
| dvisc | 0.0005438 | Paxs | 474.55 | Joback Method |
| dvisc | 0.0003651 | Paxs | 521.01 | Joback Method |
| dvisc | 0.0002617 | Paxs | 567.47 | Joback Method |
| dvisc | 0.0001973 | Paxs | 613.94 | Joback Method |
| dvisc | 0.0001547 | Paxs | 660.40 | Joback Method |

## Sources

|                        |                                                                                                                                             |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| <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>                           |
| <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=C3905644&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3905644&amp;Units=SI</a> |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <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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