

# Naphthalene, 1,2,4,6,7-pentamethyl

|                      |                                                                       |
|----------------------|-----------------------------------------------------------------------|
| Inchi:               | InChI=1S/C15H18/c1-9-7-14-12(4)6-11(3)13(5)15(14)8-10(9)2/h6-8H,1-5H3 |
| InchiKey:            | VDMSONZJLIHRGZ-UHFFFAOYSA-N                                           |
| Formula:             | C15H18                                                                |
| SMILES:              | Cc1cc2c(C)cc(C)c(C)c2cc1C                                             |
| Mol. weight [g/mol]: | 198.30                                                                |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 246.33  | kJ/mol  | Joback Method  |
| hf            | 17.32   | kJ/mol  | Joback Method  |
| hfus          | 23.72   | kJ/mol  | Joback Method  |
| hvap          | 56.21   | kJ/mol  | Joback Method  |
| log10ws       | -5.65   |         | Crippen Method |
| logp          | 4.382   |         | Crippen Method |
| mcvol         | 178.990 | ml/mol  | McGowan Method |
| pc            | 2149.31 | kPa     | Joback Method  |
| rinpol        | 308.89  |         | NIST Webbook   |
| rinpol        | 306.58  |         | NIST Webbook   |
| ripol         | 278.78  |         | NIST Webbook   |
| tb            | 613.16  | K       | Joback Method  |
| tc            | 835.07  | K       | Joback Method  |
| tf            | 380.53  | K       | Joback Method  |
| vc            | 0.690   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 437.97 | J/mol×K | 613.16          | Joback Method |
| cpg           | 454.18 | J/mol×K | 650.14          | Joback Method |
| cpg           | 469.48 | J/mol×K | 687.13          | Joback Method |
| cpg           | 483.90 | J/mol×K | 724.11          | Joback Method |
| cpg           | 497.51 | J/mol×K | 761.10          | Joback Method |
| cpg           | 510.34 | J/mol×K | 798.08          | Joback Method |
| cpg           | 522.44 | J/mol×K | 835.07          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0008508 | Pa×s | 380.53 | Joback Method |
| dvisc | 0.0006352 | Pa×s | 419.30 | Joback Method |
| dvisc | 0.0004983 | Pa×s | 458.07 | Joback Method |
| dvisc | 0.0004060 | Pa×s | 496.85 | Joback Method |
| dvisc | 0.0003408 | Pa×s | 535.62 | Joback Method |
| dvisc | 0.0002929 | Pa×s | 574.39 | Joback Method |
| dvisc | 0.0002566 | Pa×s | 613.16 | 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=R549170&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R549170&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>rinpol:</b>  | Non-polar retention indices                     |
| <b>ripol:</b>   | Polar retention indices                         |
| <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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