

# 1,1,5,6-Tetramethyl-1,2-dihydronaphthalene

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C14H18/c1-10-7-8-13-12(11(10)2)6-5-9-14(13,3)4/h5-8H,9H2,1-4H3 |
| <b>InchiKey:</b>            | WVVRPGLEZQJUSX-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C14H18  |
| <b>SMILES:</b>              | <chem>Cc1ccc2c(c1C)C=CCC2(C)C</chem>                                    |
| <b>Mol. weight [g/mol]:</b> | 186.29  |
| <b>CAS:</b>                 | 220766-68-7   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 223.64  | kJ/mol  | Joback Method  |
| hf            | 9.49    | kJ/mol  | Joback Method  |
| hfus          | 15.85   | kJ/mol  | Joback Method  |
| hvap          | 50.25   | kJ/mol  | Joback Method  |
| log10ws       | -4.45   |         | Crippen Method |
| logp          | 3.998   |         | Crippen Method |
| mcvol         | 169.200 | ml/mol  | McGowan Method |
| pc            | 2402.92 | kPa     | Joback Method  |
| rinpol        | 1486.00 |         | NIST Webbook   |
| rinpol        | 1486.00 |         | NIST Webbook   |
| rinpol        | 1511.10 |         | NIST Webbook   |
| rinpol        | 1511.10 |         | NIST Webbook   |
| ripol         | 1963.00 |         | NIST Webbook   |
| tb            | 571.75  | K       | Joback Method  |
| tc            | 801.68  | K       | Joback Method  |
| tf            | 350.60  | K       | Joback Method  |
| vc            | 0.644   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 409.62 | J/molxK | 571.75          | Joback Method |
| cpg           | 427.38 | J/molxK | 610.07          | Joback Method |
| cpg           | 444.00 | J/molxK | 648.39          | Joback Method |
| cpg           | 459.65 | J/molxK | 686.72          | Joback Method |

|     |        |         |        |               |
|-----|--------|---------|--------|---------------|
| cpg | 474.48 | J/mol×K | 725.04 | Joback Method |
| cpg | 488.66 | J/mol×K | 763.36 | Joback Method |
| cpg | 502.35 | J/mol×K | 801.68 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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=C220766687&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C220766687&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>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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