

# NAPHTHALENE, 1,2,3,4-TETRAHYDRO-5,6,7,8-TETRAMETHYL-

|                      |                                                                     |
|----------------------|---------------------------------------------------------------------|
| Other names:         | 5,6,7,8-Tetramethyl-1,2,3,4-tetrahydronaphthalene                   |
| Inchi:               | InChI=1S/C14H20/c1-9-10(2)12(4)14-8-6-5-7-13(14)11(9)3/h5-8H2,1-4H3 |
| InchiKey:            | OPDGWSYNXPRREB-UHFFFAOYSA-N                                         |
| Formula:             | C14H20                                                              |
| SMILES:              | Cc1c(C)c(C)c2c(c1C)CCCC2                                            |
| Mol. weight [g/mol]: | 188.31                                                              |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| hf            | -58.21  | kJ/mol | Cheméo Relay (1.0) |
| hfus          | 19.08   | kJ/mol | Joback Method      |
| hvap          | 71.92   | kJ/mol | Cheméo Relay (1.0) |
| ie            | 7.94    | eV     | Cheméo Relay (1.0) |
| logp          | 3.799   |        | Crippen Method     |
| mcvol         | 173.500 | ml/mol | McGowan Method     |
| rinpol        | 1602.00 |        | NIST Webbook       |
| tb            | 560.40  | K      | Cheméo Relay (1.0) |
| tf            | 423.21  | K      | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 429.68    | J/mol×K | 586.98          | Joback Method |
| cpg           | 447.78    | J/mol×K | 623.79          | Joback Method |
| cpg           | 464.87    | J/mol×K | 660.59          | Joback Method |
| cpg           | 480.99    | J/mol×K | 697.40          | Joback Method |
| cpg           | 496.19    | J/mol×K | 734.20          | Joback Method |
| cpg           | 510.51    | J/mol×K | 771.01          | Joback Method |
| cpg           | 524.00    | J/mol×K | 807.82          | Joback Method |
| dvisc         | 0.0011632 | Pa×s    | 355.22          | Joback Method |
| dvisc         | 0.0008011 | Pa×s    | 393.85          | Joback Method |
| dvisc         | 0.0005897 | Pa×s    | 432.47          | Joback Method |
| dvisc         | 0.0004564 | Pa×s    | 471.10          | Joback Method |
| dvisc         | 0.0003673 | Pa×s    | 509.73          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003047 | Pa×s | 548.35 | Joback Method |
| dvisc | 0.0002591 | Pa×s | 586.98 | Joback Method |

## Sources

|                                  |                                                                                                                                               |
|----------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C19063117&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19063117&amp;Units=SI</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>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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                             |
| <b>Cheméo Relay (1.0):</b>       |                                                                                                                                               |
| <b>Cheméo Relay (1.0, beta):</b> |                                                                                                                                               |

## Legend

|                |                                                 |
|----------------|-------------------------------------------------|
| <b>cpg:</b>    | Ideal gas heat capacity                         |
| <b>dvisc:</b>  | Dynamic viscosity                               |
| <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>ie:</b>     | Ionization energy                               |
| <b>logp:</b>   | Octanol/Water partition coefficient             |
| <b>mcvol:</b>  | McGowan's characteristic volume                 |
| <b>rinpol:</b> | Non-polar retention indices                     |
| <b>tb:</b>     | Normal Boiling Point Temperature                |
| <b>tf:</b>     | Normal melting (fusion) point                   |

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