

# Tetradecane, 2,5-dimethyl-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | 2,5-Dimethyltetradecane  |
| <b>Inchi:</b>               | InChI=1S/C16H34/c1-5-6-7-8-9-10-11-12-16(4)14-13-15(2)3/h15-16H,5-14H2,1-4H3 |
| <b>InchiKey:</b>            | RQSUKZIRUMCUSU-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C16H34   |
| <b>SMILES:</b>              | CCCCCCCCC(C)CCC(C)C  |
| <b>Mol. weight [g/mol]:</b> | 226.44   |
| <b>CAS:</b>                 | 56292-69-4   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 78.96   | kJ/mol               | Joback Method  |
| hf            | -384.13 | kJ/mol               | Joback Method  |
| hfus          | 30.15   | kJ/mol               | Joback Method  |
| hvap          | 50.43   | kJ/mol               | Joback Method  |
| log10ws       | -6.04   |                      | Crippen Method |
| logp          | 6.199   |                      | Crippen Method |
| mcvol         | 236.300 | ml/mol               | McGowan Method |
| pc            | 1333.93 | kPa                  | Joback Method  |
| tb            | 564.60  | K                    | Joback Method  |
| tc            | 728.45  | K                    | Joback Method  |
| tf            | 240.08  | K                    | Joback Method  |
| vc            | 0.919   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 612.18    | J/molxK | 564.60          | Joback Method |
| cpg           | 632.06    | J/molxK | 591.91          | Joback Method |
| cpg           | 651.14    | J/molxK | 619.22          | Joback Method |
| cpg           | 669.44    | J/molxK | 646.53          | Joback Method |
| cpg           | 686.99    | J/molxK | 673.83          | Joback Method |
| cpg           | 703.80    | J/molxK | 701.14          | Joback Method |
| cpg           | 719.89    | J/molxK | 728.45          | Joback Method |
| dvisc         | 0.0124242 | Paxs    | 240.08          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0029159 | Paxs | 294.17 | Joback Method |
| dvisc | 0.0010735 | Paxs | 348.25 | Joback Method |
| dvisc | 0.0005170 | Paxs | 402.34 | Joback Method |
| dvisc | 0.0002961 | Paxs | 456.43 | Joback Method |
| dvisc | 0.0001908 | Paxs | 510.51 | Joback Method |
| dvisc | 0.0001338 | Paxs | 564.60 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C56292694&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C56292694&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>                                     |
| <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>                         |

## 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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