

# 5,15-dimethyltrtriacontane

|                             |                                                                                  |
|-----------------------------|----------------------------------------------------------------------------------|
| <b>Inchi:</b>               | InChI=1S/C35H72/c1-5-7-9-10-11-12-13-14-15-16-17-18-19-21-24-28-32-35(4)33-29-26 |
| <b>InchiKey:</b>            | VNIMJOOGEFDUEB-UHFFFAOYSA-N                                                      |
| <b>Formula:</b>             | C35H72                                                                           |
| <b>SMILES:</b>              | CCCCCCCCCCCCCCCCCCC(C)CCCCCCCCC(C)CCCC                                           |
| <b>Mol. weight [g/mol]:</b> | 492.95                                                                           |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 238.94  | kJ/mol               | Joback Method  |
| hf            | -776.29 | kJ/mol               | Joback Method  |
| hfus          | 79.36   | kJ/mol               | Joback Method  |
| hvap          | 92.73   | kJ/mol               | Joback Method  |
| log10ws       | -13.99  |                      | Crippen Method |
| logp          | 13.611  |                      | Crippen Method |
| mvol          | 504.010 | ml/mol               | McGowan Method |
| pc            | 480.50  | kPa                  | Joback Method  |
| rinpol        | 3383.00 |                      | NIST Webbook   |
| rinpol        | 3383.00 |                      | NIST Webbook   |
| tb            | 999.32  | K                    | Joback Method  |
| tc            | 1260.43 | K                    | Joback Method  |
| tf            | 454.21  | K                    | Joback Method  |
| vc            | 1.984   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1825.56   | J/molxK | 999.32          | Joback Method |
| cpg           | 1858.31   | J/molxK | 1042.84         | Joback Method |
| cpg           | 1888.72   | J/molxK | 1086.36         | Joback Method |
| cpg           | 1916.96   | J/molxK | 1129.87         | Joback Method |
| cpg           | 1943.25   | J/molxK | 1173.39         | Joback Method |
| cpg           | 1967.79   | J/molxK | 1216.91         | Joback Method |
| cpg           | 1990.77   | J/molxK | 1260.43         | Joback Method |
| dvisc         | 0.0007702 | Paxs    | 454.21          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001994 | Paxs | 545.06 | Joback Method |
| dvisc | 0.0000760 | Paxs | 635.91 | Joback Method |
| dvisc | 0.0000368 | Paxs | 726.76 | Joback Method |
| dvisc | 0.0000210 | Paxs | 817.62 | Joback Method |
| dvisc | 0.0000134 | Paxs | 908.47 | Joback Method |
| dvisc | 0.0000093 | Paxs | 999.32 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R272558&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R272558&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>rinpol:</b>  | Non-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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