

# 3,3-Diethylpentadecane

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C19H40/c1-5-9-10-11-12-13-14-15-16-17-18-19(6-2,7-3)8-4/h5-18H2,1-4H3 |
| <b>InchiKey:</b>            | FUFJQEHAHXDXFH-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C19H40   |
| <b>SMILES:</b>              | CCCCCCCCCCCC(CC)(CC)CC   |
| <b>Mol. weight [g/mol]:</b> | 268.52   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 111.94  | kJ/mol               | Joback Method  |
| hf            | -444.24 | kJ/mol               | Joback Method  |
| hfus          | 37.55   | kJ/mol               | Joback Method  |
| hvap          | 56.59   | kJ/mol               | Joback Method  |
| log10ws       | -7.53   |                      | Crippen Method |
| logp          | 7.514   |                      | Crippen Method |
| mvol          | 278.570 | ml/mol               | McGowan Method |
| pc            | 1094.27 | kPa                  | Joback Method  |
| rinpol        | 1857.00 |                      | NIST Webbook   |
| rinpol        | 1857.00 |                      | NIST Webbook   |
| tb            | 630.89  | K                    | Joback Method  |
| tc            | 795.73  | K                    | Joback Method  |
| tf            | 306.31  | K                    | Joback Method  |
| vc            | 1.089   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 783.43    | J/molxK | 630.89          | Joback Method |
| cpg           | 804.55    | J/molxK | 658.36          | Joback Method |
| cpg           | 824.75    | J/molxK | 685.84          | Joback Method |
| cpg           | 844.05    | J/molxK | 713.31          | Joback Method |
| cpg           | 862.50    | J/molxK | 740.78          | Joback Method |
| cpg           | 880.12    | J/molxK | 768.26          | Joback Method |
| cpg           | 896.96    | J/molxK | 795.73          | Joback Method |
| dvisc         | 0.0048700 | Paxs    | 306.31          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0015472 | Paxs | 360.41 | Joback Method |
| dvisc | 0.0006630 | Paxs | 414.50 | Joback Method |
| dvisc | 0.0003455 | Paxs | 468.60 | Joback Method |
| dvisc | 0.0002061 | Paxs | 522.70 | Joback Method |
| dvisc | 0.0001354 | Paxs | 576.79 | Joback Method |
| dvisc | 0.0000956 | Paxs | 630.89 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U360411&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360411&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>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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