

# Hexadecane, 5-propyl

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C19H40/c1-4-7-9-10-11-12-13-14-15-18-19(16-6-3)17-8-5-2/h19H,4-18H2,1-3H |
| <b>InchiKey:</b>            | HAWQMXBQEHSBHU-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C19H40  |
| <b>SMILES:</b>              | CCCCCCCCCCCC(CCC)CCCC   |
| <b>Mol. weight [g/mol]:</b> | 268.52  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 106.66  | kJ/mol               | Joback Method  |
| hf            | -440.77 | kJ/mol               | Joback Method  |
| hfus          | 41.44   | kJ/mol               | Joback Method  |
| hvap          | 57.50   | kJ/mol               | Joback Method  |
| log10ws       | -7.53   |                      | Crippen Method |
| logp          | 7.514   |                      | Crippen Method |
| mcvol         | 278.570 | ml/mol               | McGowan Method |
| pc            | 1086.35 | kPa                  | Joback Method  |
| rinsol        | 1809.00 |                      | NIST Webbook   |
| tb            | 633.68  | K                    | Joback Method  |
| tc            | 794.96  | K                    | Joback Method  |
| tf            | 288.89  | K                    | Joback Method  |
| vc            | 1.093   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 781.70    | J/molxK | 633.68          | Joback Method |
| cpg           | 877.35    | J/molxK | 768.08          | Joback Method |
| cpg           | 859.82    | J/molxK | 741.20          | Joback Method |
| cpg           | 841.51    | J/molxK | 714.32          | Joback Method |
| cpg           | 822.41    | J/molxK | 687.44          | Joback Method |
| cpg           | 802.48    | J/molxK | 660.56          | Joback Method |
| cpg           | 894.13    | J/molxK | 794.96          | Joback Method |
| dvisc         | 0.0001019 | Paxs    | 633.68          | Joback Method |
| dvisc         | 0.0001427 | Paxs    | 576.22          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0002152 | Paxs | 518.75 | Joback Method |
| dvisc | 0.0003595 | Paxs | 461.29 | Joback Method |
| dvisc | 0.0006952 | Paxs | 403.82 | Joback Method |
| dvisc | 0.0016729 | Paxs | 346.36 | Joback Method |
| dvisc | 0.0057089 | Paxs | 288.89 | 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=R47853&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R47853&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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