

# Eicosane, 10-hexyl-10-methyl-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 10-Hexyl-10-methyleicosane  |
| <b>Inchi:</b>               | InChI=1S/C27H56/c1-5-8-11-14-16-18-20-23-26-27(4,24-21-13-10-7-3)25-22-19-17-15-1 |
| <b>InchiKey:</b>            | SHJTUYDWGDNRHW-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C27H56  |
| <b>SMILES:</b>              | CCCCCCCCCCC(C)(CCCCCC)CCCCCCCCC   |
| <b>Mol. weight [g/mol]:</b> | 380.73  |
| <b>CAS:</b>                 | 55282-32-1  |

## Physical Properties

| Property code | Value         | Unit                 | Source         |
|---------------|---------------|----------------------|----------------|
| gf            | 179.30        | kJ/mol               | Joback Method  |
| hf            | -609.36       | kJ/mol               | Joback Method  |
| hfus          | 58.27         | kJ/mol               | Joback Method  |
| hvap          | 129.90 ± 1.80 | kJ/mol               | NIST Webbook   |
| log10ws       | -10.88        |                      | Crippen Method |
| logp          | 10.635        |                      | Crippen Method |
| mcvol         | 391.290       | ml/mol               | McGowan Method |
| pc            | 695.81        | kPa                  | Joback Method  |
| tb            | 813.93        | K                    | Joback Method  |
| tc            | 996.49        | K                    | Joback Method  |
| tf            | 188.00 ± 3.00 | K                    | NIST Webbook   |
| vc            | 1.536         | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1282.03   | J/mol×K | 813.93          | Joback Method |
| cpg           | 1306.42   | J/mol×K | 844.36          | Joback Method |
| cpg           | 1329.60   | J/mol×K | 874.78          | Joback Method |
| cpg           | 1351.65   | J/mol×K | 905.21          | Joback Method |
| cpg           | 1372.63   | J/mol×K | 935.64          | Joback Method |
| cpg           | 1392.59   | J/mol×K | 966.07          | Joback Method |
| cpg           | 1411.62   | J/mol×K | 996.49          | Joback Method |
| dvisc         | 0.0016537 | Paxs    | 396.47          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0005159 | Paxs | 466.05 | Joback Method |
| dvisc | 0.0002178 | Paxs | 535.62 | Joback Method |
| dvisc | 0.0001122 | Paxs | 605.20 | Joback Method |
| dvisc | 0.0000662 | Paxs | 674.78 | Joback Method |
| dvisc | 0.0000431 | Paxs | 744.35 | Joback Method |
| dvisc | 0.0000302 | Paxs | 813.93 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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=C55282321&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55282321&amp;Units=SI</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>                                     |

## Legend

|                                       |   |
|---------------------------------------|---|
| <b>cp<sub>g</sub>:</b>                | Ideal gas heat capacity                         |
| <b>dvisc:</b>                         | Dynamic viscosity                               |
| <b>g<sub>f</sub>:</b>                 | Standard Gibbs free energy of formation         |
| <b>h<sub>f</sub>:</b>                 | Enthalpy of formation at standard conditions    |
| <b>h<sub>fus</sub>:</b>               | Enthalpy of fusion at standard conditions       |
| <b>h<sub>vap</sub>:</b>               | Enthalpy of vaporization at standard conditions |
| <b>log<sub>10</sub>w<sub>s</sub>:</b> | Log <sub>10</sub> of Water solubility in mol/l  |
| <b>log<sub>p</sub>:</b>               | Octanol/Water partition coefficient             |
| <b>mc<sub>vol</sub>:</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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