

# Tridecane, 6-ethyl

|                      |                                                                        |
|----------------------|------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C15H32/c1-4-7-9-10-12-14-15(6-3)13-11-8-5-2/h15H,4-14H2,1-3H3 |
| InchiKey:            | VPFNFUHSGMMEIA-UHFFFAOYSA-N                                            |
| Formula:             | C15H32                                                                 |
| SMILES:              | CCCCCCCC(CC)CCCCC                                                      |
| Mol. weight [g/mol]: | 212.41                                                                 |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 72.98   | kJ/mol  | Joback Method  |
| hf            | -358.21 | kJ/mol  | Joback Method  |
| hfus          | 31.08   | kJ/mol  | Joback Method  |
| hvap          | 48.60   | kJ/mol  | Joback Method  |
| log10ws       | -5.86   |         | Crippen Method |
| logp          | 5.953   |         | Crippen Method |
| mcvol         | 222.210 | ml/mol  | McGowan Method |
| pc            | 1423.99 | kPa     | Joback Method  |
| rinpol        | 1424.00 |         | NIST Webbook   |
| rinpol        | 1424.00 |         | NIST Webbook   |
| tb            | 542.16  | K       | Joback Method  |
| tc            | 703.93  | K       | Joback Method  |
| tf            | 243.81  | K       | Joback Method  |
| vc            | 0.870   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 558.22    | J/mol×K | 542.16          | Joback Method |
| cpg           | 577.24    | J/mol×K | 569.12          | Joback Method |
| cpg           | 595.52    | J/mol×K | 596.08          | Joback Method |
| cpg           | 613.07    | J/mol×K | 623.04          | Joback Method |
| cpg           | 629.92    | J/mol×K | 650.00          | Joback Method |
| cpg           | 646.08    | J/mol×K | 676.97          | Joback Method |
| cpg           | 661.59    | J/mol×K | 703.93          | Joback Method |
| dvisc         | 0.0083877 | Pa×s    | 243.81          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0024681 | Pa×s | 293.53 | Joback Method |
| dvisc | 0.0010352 | Pa×s | 343.26 | Joback Method |
| dvisc | 0.0005409 | Pa×s | 392.99 | Joback Method |
| dvisc | 0.0003270 | Pa×s | 442.71 | Joback Method |
| dvisc | 0.0002189 | Pa×s | 492.43 | Joback Method |
| dvisc | 0.0001577 | Pa×s | 542.16 | 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=R9880&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R9880&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>10ws</sub>:</b> | Log10 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>p<sub>c</sub>:</b>      | Critical Pressure                               |
| <b>ri<sub>pol</sub>:</b>   | Non-polar retention indices                     |
| <b>t<sub>b</sub>:</b>      | Normal Boiling Point Temperature                |
| <b>t<sub>c</sub>:</b>      | Critical Temperature                            |
| <b>t<sub>f</sub>:</b>      | Normal melting (fusion) point                   |
| <b>v<sub>c</sub>:</b>      | Critical Volume                                 |

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