

# Tridecane, 7-ethyl-6-propyl

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C18H38/c1-5-9-11-13-15-17(8-4)18(14-7-3)16-12-10-6-2/h17-18H,5-16H2,1-4H |
| <b>InchiKey:</b>            | CLJKRTSBRZETFQ-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C18H38  |
| <b>SMILES:</b>              | CCCCCCC(CC)C(CCC)CCCCC  |
| <b>Mol. weight [g/mol]:</b> | 254.49  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 95.80   | kJ/mol  | Joback Method  |
| hf            | -425.41 | kJ/mol  | Joback Method  |
| hfus          | 35.33   | kJ/mol  | Joback Method  |
| hvap          | 54.89   | kJ/mol  | Joback Method  |
| log10ws       | -6.87   |         | Crippen Method |
| logp          | 6.980   |         | Crippen Method |
| mcvol         | 264.480 | ml/mol  | McGowan Method |
| pc            | 1164.84 | kPa     | Joback Method  |
| rinpol        | 1592.00 |         | NIST Webbook   |
| rinpol        | 1592.00 |         | NIST Webbook   |
| tb            | 610.36  | K       | Joback Method  |
| tc            | 773.50  | K       | Joback Method  |
| tf            | 262.62  | K       | Joback Method  |
| vc            | 1.032   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 724.07    | J/molxK | 610.36          | Joback Method |
| cpg           | 819.32    | J/molxK | 746.31          | Joback Method |
| cpg           | 801.88    | J/molxK | 719.12          | Joback Method |
| cpg           | 783.65    | J/molxK | 691.93          | Joback Method |
| cpg           | 764.63    | J/molxK | 664.74          | Joback Method |
| cpg           | 744.77    | J/molxK | 637.55          | Joback Method |
| cpg           | 836.01    | J/molxK | 773.50          | Joback Method |
| dvisc         | 0.0001069 | Paxs    | 610.36          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001529 | Paxs | 552.40 | Joback Method |
| dvisc | 0.0002378 | Paxs | 494.45 | Joback Method |
| dvisc | 0.0004158 | Paxs | 436.49 | Joback Method |
| dvisc | 0.0008629 | Paxs | 378.53 | Joback Method |
| dvisc | 0.0023312 | Paxs | 320.58 | Joback Method |
| dvisc | 0.0097660 | Paxs | 262.62 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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=R9940&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R9940&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>                                 |

## Legend

|                            |   |
|----------------------------|---|
| <b>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b> | Log <sub>10</sub> 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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