

# 4-Propyldecane

|                      |                                                                  |
|----------------------|------------------------------------------------------------------|
| Inchi:               | InChI=1S/C13H28/c1-4-7-8-9-12-13(10-5-2)11-6-3/h13H,4-12H2,1-3H3 |
| InchiKey:            | DEYIWSIHCYZIOF-UHFFFAOYSA-N                                      |
| Formula:             | C13H28                                                           |
| SMILES:              | CCCCCCC(CCC)CCC                                                  |
| Mol. weight [g/mol]: | 184.37                                                           |

## Physical Properties

| Property code | Value   | Unit    | Source             |
|---------------|---------|---------|--------------------|
| af            | 0.5575  |         | Cheméo Relay (1.0) |
| gf            | 56.14   | kJ/mol  | Joback Method      |
| hf            | -302.50 | kJ/mol  | Cheméo Relay (1.0) |
| hfus          | 25.90   | kJ/mol  | Joback Method      |
| hvap          | 58.46   | kJ/mol  | Cheméo Relay (1.0) |
| ie            | 9.31    | eV      | Cheméo Relay (1.0) |
| log10ws       | -6.62   |         | Cheméo Relay (1.0) |
| logp          | 5.173   |         | Crippen Method     |
| mcvol         | 194.030 | ml/mol  | McGowan Method     |
| pc            | 1655.15 | kPa     | Joback Method      |
| rinpol        | 1220.00 |         | NIST Webbook       |
| rinpol        | 1222.00 |         | NIST Webbook       |
| tb            | 492.22  | K       | Cheméo Relay (1.0) |
| tc            | 657.09  | K       | Cheméo Relay (1.0) |
| tf            | 209.55  | K       | Cheméo Relay (1.0) |
| vc            | 0.727   | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 455.59 | J/mol×K | 496.40          | Joback Method |
| cpg           | 552.81 | J/mol×K | 659.72          | Joback Method |
| cpg           | 538.20 | J/mol×K | 632.50          | Joback Method |
| cpg           | 522.98 | J/mol×K | 605.28          | Joback Method |
| cpg           | 507.13 | J/mol×K | 578.06          | Joback Method |
| cpg           | 490.62 | J/mol×K | 550.84          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 473.45    | J/mol×K | 523.62 | Joback Method |
| dvisc | 0.0006335 | Pa×s    | 358.83 | Joback Method |
| dvisc | 0.0001881 | Pa×s    | 496.40 | Joback Method |
| dvisc | 0.0002596 | Pa×s    | 450.54 | Joback Method |
| dvisc | 0.0003856 | Pa×s    | 404.69 | Joback Method |
| dvisc | 0.0096568 | Pa×s    | 221.27 | Joback Method |
| dvisc | 0.0012038 | Pa×s    | 312.98 | Joback Method |
| dvisc | 0.0028515 | Pa×s    | 267.12 | Joback Method |

## Sources

|                                  |                                                                                                                                       |
|----------------------------------|---------------------------------------------------------------------------------------------------------------------------------------|
| <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>                             |
| <b>Crippen Method:</b>           | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                     |
| <b>Cheméo Relay (1.0):</b>       |                                                                                                                                       |
| <b>Cheméo Relay (1.0, beta):</b> |                                                                                                                                       |
| <b>NIST Webbook:</b>             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R8907&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R8907&amp;Units=SI</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>                 |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>af:</b>      | Acentric Factor                                 |
| <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>ie:</b>      | Ionization energy                               |
| <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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