

# Cyclohexane, eicosyl-

|                      |                                                                                    |
|----------------------|------------------------------------------------------------------------------------|
| Other names:         | Eicosane, 1-cyclohexyl-<br>1-Cyclohexyleicosane<br>n-Eicosylcyclohexane            |
| Inchi:               | InChI=1S/C26H52/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-20-23-26-24-21-19-22 |
| InchiKey:            | PSPNTGGVAYLSJO-UHFFFAOYSA-N                                                        |
| Formula:             | C26H52                                                                             |
| SMILES:              | CCCCCCCCCCCCCCCCCCCC1CCCCC1                                                        |
| Mol. weight [g/mol]: | 364.69                                                                             |
| CAS:                 | 4443-55-4                                                                          |

## Physical Properties

| Property code | Value         | Unit    | Source         |
|---------------|---------------|---------|----------------|
| gf            | 192.49        | kJ/mol  | Joback Method  |
| hf            | -525.65       | kJ/mol  | Joback Method  |
| hfus          | 54.93         | kJ/mol  | Joback Method  |
| hvap          | 73.90         | kJ/mol  | Joback Method  |
| log10ws       | -10.36        |         | Crippen Method |
| logp          | 9.998         |         | Crippen Method |
| mcvol         | 366.340       | ml/mol  | McGowan Method |
| pc            | 812.14        | kPa     | Joback Method  |
| tb            | 813.83        | K       | Joback Method  |
| tc            | 999.07        | K       | Joback Method  |
| tf            | 321.05 ± 0.50 | K       | NIST Webbook   |
| tf            | 321.05 ± 1.50 | K       | NIST Webbook   |
| vc            | 1.425         | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1217.53 | J/mol×K | 813.83          | Joback Method |
| cpg           | 1241.93 | J/mol×K | 844.70          | Joback Method |
| cpg           | 1265.01 | J/mol×K | 875.58          | Joback Method |
| cpg           | 1286.82 | J/mol×K | 906.45          | Joback Method |
| cpg           | 1307.43 | J/mol×K | 937.32          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 1326.88   | J/mol×K | 968.20 | Joback Method |
| cpg   | 1345.23   | J/mol×K | 999.07 | Joback Method |
| dvisc | 0.0021271 | Pa×s    | 390.16 | Joback Method |
| dvisc | 0.0006855 | Pa×s    | 460.77 | Joback Method |
| dvisc | 0.0002985 | Pa×s    | 531.38 | Joback Method |
| dvisc | 0.0001580 | Pa×s    | 601.99 | Joback Method |
| dvisc | 0.0000956 | Pa×s    | 672.61 | Joback Method |
| dvisc | 0.0000636 | Pa×s    | 743.22 | Joback Method |
| dvisc | 0.0000454 | Pa×s    | 813.83 | Joback Method |
| hvapt | 94.20     | kJ/mol  | 518.50 | NIST Webbook  |

## Sources

|                        |                                                                                                                                             |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4443554&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4443554&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>                                   |
| <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>                       |

## 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>hvapt:</b>   | Enthalpy of vaporization at a given temperature |
| <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>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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