

# Cyclopentane, heneicosyl-

|                      |                                                                                    |
|----------------------|------------------------------------------------------------------------------------|
| Other names:         | Heneicosane, 1-cyclopentyl-n-Heneicosylcyclopentane                                |
| Inchi:               | InChI=1S/C26H52/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-26-24-21-22 |
| InchiKey:            | GNECQVKDNNGLCG-UHFFFAOYSA-N                                                        |
| Formula:             | C26H52                                                                             |
| SMILES:              | CCCCCCCCCCCCCCCCCCCCCCCC1CCCC1                                                     |
| Mol. weight [g/mol]: | 364.69                                                                             |
| CAS:                 | 6703-82-8                                                                          |

## Physical Properties

| Property code | Value            | Unit    | Source         |
|---------------|------------------|---------|----------------|
| chl           | -17014.20 ± 6.70 | kJ/mol  | NIST Webbook   |
| gf            | 204.59           | kJ/mol  | Joback Method  |
| hf            | -519.49          | kJ/mol  | Joback Method  |
| hfl           | -648.60 ± 6.70   | kJ/mol  | NIST Webbook   |
| hfus          | 57.03            | kJ/mol  | Joback Method  |
| hvap          | 73.73            | kJ/mol  | Joback Method  |
| log10ws       | -10.36           |         | Crippen Method |
| logp          | 9.998            |         | Crippen Method |
| mcvol         | 366.340          | ml/mol  | McGowan Method |
| pc            | 800.69           | kPa     | Joback Method  |
| rinpol        | 2691.00          |         | NIST Webbook   |
| tb            | 809.56           | K       | Joback Method  |
| tc            | 992.90           | K       | Joback Method  |
| tf            | 45.20 ± 1.50     | K       | NIST Webbook   |
| tf            | 318.40 ± 1.00    | K       | NIST Webbook   |
| tf            | 318.35 ± 0.50    | K       | NIST Webbook   |
| vc            | 1.433            | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1339.83 | J/mol×K | 992.90          | Joback Method |
| cpg           | 1212.39 | J/mol×K | 809.56          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 1236.55   | J/mol×K | 840.12 | Joback Method |
| cpg   | 1259.47   | J/mol×K | 870.67 | Joback Method |
| cpg   | 1281.19   | J/mol×K | 901.23 | Joback Method |
| cpg   | 1301.79   | J/mol×K | 931.79 | Joback Method |
| cpg   | 1321.32   | J/mol×K | 962.35 | Joback Method |
| dvisc | 0.0000647 | Pa×s    | 809.56 | Joback Method |
| dvisc | 0.0021080 | Pa×s    | 393.68 | Joback Method |
| dvisc | 0.0007638 | Pa×s    | 462.99 | Joback Method |
| dvisc | 0.0003605 | Pa×s    | 532.31 | Joback Method |
| dvisc | 0.0002023 | Pa×s    | 601.62 | Joback Method |
| dvisc | 0.0001279 | Pa×s    | 670.93 | Joback Method |
| dvisc | 0.0000881 | Pa×s    | 740.25 | Joback Method |
| hvapt | 93.80     | kJ/mol  | 517.50 | NIST Webbook  |

## Sources

|                        |                                                                                                                                             |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| <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=C6703828&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6703828&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>                           |

## Legend

|                 |                                                           |
|-----------------|-----------------------------------------------------------|
| <b>chl:</b>     | Standard liquid enthalpy of combustion                    |
| <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>hfl:</b>     | Liquid phase 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>mccvol:</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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