

# n-Heptadecylcyclohexane

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Other names:         | Cyclohexane, heptadecyl-<br>Heptadecylcyclohexane<br>Hexadecylcyclohexane         |
| Inchi:               | InChI=1S/C23H46/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-17-20-23-21-18-16-19-22-23/h |
| InchiKey:            | VLHZQNGNJQYIAIZ-UHFFFAOYSA-N                                                      |
| Formula:             | C23H46                                                                            |
| SMILES:              | CCCCCCCCCCCCCCCCCCCC1CCCCC1                                                       |
| Mol. weight [g/mol]: | 322.61                                                                            |
| CAS:                 | 19781-73-8                                                                        |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 167.23  | kJ/mol  | Joback Method  |
| hf            | -463.73 | kJ/mol  | Joback Method  |
| hfus          | 47.16   | kJ/mol  | Joback Method  |
| hvap          | 67.22   | kJ/mol  | Joback Method  |
| log10ws       | -9.10   |         | Crippen Method |
| logp          | 8.828   |         | Crippen Method |
| mcvol         | 324.070 | ml/mol  | McGowan Method |
| pc            | 963.87  | kPa     | Joback Method  |
| rinpol        | 372.80  |         | NIST Webbook   |
| tb            | 745.19  | K       | Joback Method  |
| tc            | 924.52  | K       | Joback Method  |
| tf            | 356.35  | K       | Joback Method  |
| vc            | 1.256   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1024.48 | J/mol×K | 745.19          | Joback Method |
| cpg           | 1048.20 | J/mol×K | 775.08          | Joback Method |
| cpg           | 1070.71 | J/mol×K | 804.97          | Joback Method |
| cpg           | 1092.06 | J/mol×K | 834.85          | Joback Method |
| cpg           | 1112.28 | J/mol×K | 864.74          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 1131.43   | J/mol×K | 894.63 | Joback Method |
| cpg   | 1149.55   | J/mol×K | 924.52 | Joback Method |
| dvisc | 0.0031190 | Pa×s    | 356.35 | Joback Method |
| dvisc | 0.0010147 | Pa×s    | 421.16 | Joback Method |
| dvisc | 0.0004454 | Pa×s    | 485.96 | Joback Method |
| dvisc | 0.0002373 | Pa×s    | 550.77 | Joback Method |
| dvisc | 0.0001444 | Pa×s    | 615.58 | Joback Method |
| dvisc | 0.0000965 | Pa×s    | 680.38 | Joback Method |
| dvisc | 0.0000692 | Pa×s    | 745.19 | Joback Method |
| hvapt | 97.60     | kJ/mol  | 539.00 | NIST Webbook  |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.49287e+01                   |
| Coeff. B                    | -5.04154e+03                  |
| Coeff. C                    | -1.60369e+02                  |
| Temperature range (K), min. | 504.71                        |
| Temperature range (K), max. | 684.59                        |

## Sources

|                                      |                                                                                                                                                                                         |
|--------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method:                      | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                                                                   |
| NIST Webbook:                        | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C19781738&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19781738&amp;Units=SI</a>                                           |
| The Yaws Handbook of Vapor Pressure: | <a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a> |
| Crippen Method:                      | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                                                               |
| Crippen Method:                      | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                                                                       |
| Joback Method:                       | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                                                                   |

## Legend

|        |                                         |
|--------|-----------------------------------------|
| cpg:   | Ideal gas heat capacity                 |
| dvisc: | Dynamic viscosity                       |
| gf:    | 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>hvac:</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>pvap:</b>    | Vapor 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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