

# 5-Methyltricosane

|                      |                                                                                    |
|----------------------|------------------------------------------------------------------------------------|
| Other names:         | Tricosane, 5-methyl                                                                |
| Inchi:               | InChI=1S/C24H50/c1-4-6-8-9-10-11-12-13-14-15-16-17-18-19-20-21-23-24(3)22-7-5-2/h2 |
| InchiKey:            | MWORWWXTNWRHAD-UHFFFAOYSA-N                                                        |
| Formula:             | C24H50                                                                             |
| SMILES:              | CCCCCCCCCCCCCCCCCCCC(C)CCCC                                                        |
| Mol. weight [g/mol]: | 338.65                                                                             |
| CAS:                 | 22331-09-5                                                                         |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| gf            | 148.76  | kJ/mol | Joback Method  |
| hf            | -543.97 | kJ/mol | Joback Method  |
| hfus          | 54.39   | kJ/mol | Joback Method  |
| hvap          | 68.63   | kJ/mol | Joback Method  |
| log10ws       | -9.63   |        | Crippen Method |
| logp          | 9.464   |        | Crippen Method |
| mcvol         | 349.020 | ml/mol | McGowan Method |
| pc            | 809.83  | kPa    | Joback Method  |
| rinpol        | 2352.00 |        | NIST Webbook   |
| rinpol        | 2346.30 |        | NIST Webbook   |
| rinpol        | 2350.00 |        | NIST Webbook   |
| rinpol        | 2348.00 |        | NIST Webbook   |
| rinpol        | 2349.00 |        | NIST Webbook   |
| rinpol        | 2352.00 |        | NIST Webbook   |
| rinpol        | 2347.00 |        | NIST Webbook   |
| rinpol        | 2352.00 |        | NIST Webbook   |
| rinpol        | 2352.90 |        | NIST Webbook   |
| rinpol        | 2351.00 |        | NIST Webbook   |
| rinpol        | 2354.00 |        | NIST Webbook   |
| rinpol        | 2346.00 |        | NIST Webbook   |
| rinpol        | 2351.00 |        | NIST Webbook   |
| rinpol        | 2349.00 |        | NIST Webbook   |
| ripol         | 2348.70 |        | NIST Webbook   |
| ripol         | 2348.70 |        | NIST Webbook   |
| tb            | 748.08  | K      | Joback Method  |
| tc            | 918.22  | K      | Joback Method  |
| tf            | 345.24  | K      | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1087.86   | J/mol×K | 748.08          | Joback Method |
| cpg           | 1110.78   | J/mol×K | 776.44          | Joback Method |
| cpg           | 1132.66   | J/mol×K | 804.79          | Joback Method |
| cpg           | 1153.54   | J/mol×K | 833.15          | Joback Method |
| cpg           | 1173.45   | J/mol×K | 861.51          | Joback Method |
| cpg           | 1192.43   | J/mol×K | 889.86          | Joback Method |
| cpg           | 1210.52   | J/mol×K | 918.22          | Joback Method |
| dvisc         | 0.0031119 | Pa×s    | 345.24          | Joback Method |
| dvisc         | 0.0009096 | Pa×s    | 412.38          | Joback Method |
| dvisc         | 0.0003752 | Pa×s    | 479.52          | Joback Method |
| dvisc         | 0.0001924 | Pa×s    | 546.66          | Joback Method |
| dvisc         | 0.0001142 | Pa×s    | 613.80          | Joback Method |
| dvisc         | 0.0000751 | Pa×s    | 680.94          | Joback Method |
| dvisc         | 0.0000532 | Pa×s    | 748.08          | Joback Method |
| hvapt         | 79.60     | kJ/mol  | 578.00          | NIST Webbook  |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.89936e+01                   |
| Coeff. B                    | -9.27150e+03                  |
| Coeff. C                    | -8.29900e+00                  |
| Temperature range (K), min. | 503.94                        |
| Temperature range (K), max. | 685.94                        |

## Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C22331095&Units=SI>

**The Yaws Handbook of Vapor**

**Pressure:**  
**Crippen Method:**

**Crippen Method:**

**Joback Method:**

**McGowan Method:**

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

<http://link.springer.com/article/10.1007/BF02311772>

## 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>pvap:</b>    | Vapor pressure                                  |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>ripol:</b>   | 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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