

# 13-Methylheptatriacontane

**Inchi:** InChI=1S/C38H78/c1-4-6-8-10-12-14-16-17-18-19-20-21-22-23-24-25-26-27-29-31-33-35  
**InchiKey:** XBGZSXCMVDZHG-UHFFFAOYSA-N  
**Formula:** C38H78  
**SMILES:** CCCCCCCCCCCCCCCCCCCCCCCCCC(C)CCCCCCCCCCCC  
**Mol. weight [g/mol]:** 535.03  
**CAS:** 56987-87-2

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 266.64  | kJ/mol               | Joback Method  |
| hf            | -832.93 | kJ/mol               | Joback Method  |
| hfus          | 90.65   | kJ/mol               | Joback Method  |
| hvap          | 99.79   | kJ/mol               | Joback Method  |
| log10ws       | -15.49  |                      | Crippen Method |
| logp          | 14.926  |                      | Crippen Method |
| mcvol         | 546.280 | ml/mol               | McGowan Method |
| pc            | 423.73  | kPa                  | Joback Method  |
| rinpol        | 3722.00 |                      | NIST Webbook   |
| rinpol        | 3735.00 |                      | NIST Webbook   |
| rinpol        | 3729.00 |                      | NIST Webbook   |
| rinpol        | 3730.00 |                      | NIST Webbook   |
| rinpol        | 3735.00 |                      | NIST Webbook   |
| rinpol        | 3730.00 |                      | NIST Webbook   |
| rinpol        | 3733.00 |                      | NIST Webbook   |
| rinpol        | 3735.00 |                      | NIST Webbook   |
| tb            | 1068.40 | K                    | Joback Method  |
| tc            | 1389.46 | K                    | Joback Method  |
| tf            | 503.02  | K                    | Joback Method  |
| vc            | 2.158   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 2035.08 | J/mol×K | 1068.40         | Joback Method |

|       |           |         |         |               |
|-------|-----------|---------|---------|---------------|
| cpg   | 2200.09   | J/molxK | 1335.95 | Joback Method |
| cpg   | 2171.93   | J/molxK | 1282.44 | Joback Method |
| cpg   | 2141.75   | J/molxK | 1228.93 | Joback Method |
| cpg   | 2109.16   | J/molxK | 1175.42 | Joback Method |
| cpg   | 2073.73   | J/molxK | 1121.91 | Joback Method |
| cpg   | 2226.65   | J/molxK | 1389.46 | Joback Method |
| dvisc | 0.0000063 | Paxs    | 1068.40 | Joback Method |
| dvisc | 0.0000089 | Paxs    | 974.17  | Joback Method |
| dvisc | 0.0000138 | Paxs    | 879.94  | Joback Method |
| dvisc | 0.0000235 | Paxs    | 785.71  | Joback Method |
| dvisc | 0.0000464 | Paxs    | 691.48  | Joback Method |
| dvisc | 0.0001137 | Paxs    | 597.25  | Joback Method |
| dvisc | 0.0003897 | Paxs    | 503.02  | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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=C56987872&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C56987872&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>   |

## 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>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                   |

**vc:** Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/40-854-9/13-Methylheptatriacontane.pdf>

Generated by Cheméo on 2024-05-01 12:51:19.121263695 +0000 UTC m=+16857128.041841010.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.