

# 5,9,13-trimethylnonacosane

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C32H66/c1-6-8-10-11-12-13-14-15-16-17-18-19-20-21-25-31(4)27-23-29-32(5) |
| <b>InchiKey:</b>            | PIOISYJJQUFRLD-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C32H66  |
| <b>SMILES:</b>              | CCCCCCCCCCCCCCCC(C)CCCC(C)CCCC(C)CCCC   |
| <b>Mol. weight [g/mol]:</b> | 450.87  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 211.24  | kJ/mol               | Joback Method  |
| hf            | -719.65 | kJ/mol               | Joback Method  |
| hfus          | 68.07   | kJ/mol               | Joback Method  |
| hvap          | 85.66   | kJ/mol               | Joback Method  |
| log10ws       | -12.49  |                      | Crippen Method |
| logp          | 12.297  |                      | Crippen Method |
| mvol          | 461.740 | ml/mol               | McGowan Method |
| pc            | 549.49  | kPa                  | Joback Method  |
| rinpol        | 3009.00 |                      | NIST Webbook   |
| rinpol        | 3009.00 |                      | NIST Webbook   |
| tb            | 930.24  | K                    | Joback Method  |
| tc            | 1150.49 | K                    | Joback Method  |
| tf            | 405.40  | K                    | Joback Method  |
| vc            | 1.810   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1618.98   | J/molxK | 930.24          | Joback Method |
| cpg           | 1647.60   | J/molxK | 966.95          | Joback Method |
| cpg           | 1674.45   | J/molxK | 1003.66         | Joback Method |
| cpg           | 1699.63   | J/molxK | 1040.36         | Joback Method |
| cpg           | 1723.25   | J/molxK | 1077.07         | Joback Method |
| cpg           | 1745.43   | J/molxK | 1113.78         | Joback Method |
| cpg           | 1766.27   | J/molxK | 1150.49         | Joback Method |
| dvisc         | 0.0016243 | Paxs    | 405.40          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003607 | Paxs | 492.87 | Joback Method |
| dvisc | 0.0001261 | Paxs | 580.35 | Joback Method |
| dvisc | 0.0000581 | Paxs | 667.82 | Joback Method |
| dvisc | 0.0000320 | Paxs | 755.29 | Joback Method |
| dvisc | 0.0000199 | Paxs | 842.77 | Joback Method |
| dvisc | 0.0000136 | Paxs | 930.24 | Joback Method |

## 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=R280316&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R280316&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>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                   |
| <b>vc:</b>      | Critical Volume                                 |

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