

# Dotriacontanal, 12-methyl

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C33H66O/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-18-21-24-27-30-33(2)31-28 |
| <b>InchiKey:</b>            | FUWIDCPSLWQYJR-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C33H66O  |
| <b>SMILES:</b>              | CCCCCCCCCCCCCCCCCCCC(C)CCCCCCCCCCC=O   |
| <b>Mol. weight [g/mol]:</b> | 478.88   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 125.02  | kJ/mol  | Joback Method  |
| hf            | -815.31 | kJ/mol  | Joback Method  |
| hfus          | 79.99   | kJ/mol  | Joback Method  |
| hvap          | 95.38   | kJ/mol  | Joback Method  |
| log10ws       | -12.67  |         | Crippen Method |
| logp          | 12.154  |         | Crippen Method |
| mcvol         | 477.400 | ml/mol  | McGowan Method |
| pc            | 539.83  | kPa     | Joback Method  |
| rinpol        | 3462.00 |         | NIST Webbook   |
| tb            | 1002.66 | K       | Joback Method  |
| tc            | 1261.41 | K       | Joback Method  |
| tf            | 488.67  | K       | Joback Method  |
| vc            | 1.895   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1715.06   | J/molxK | 1002.66         | Joback Method |
| cpg           | 1744.86   | J/molxK | 1045.78         | Joback Method |
| cpg           | 1772.51   | J/molxK | 1088.91         | Joback Method |
| cpg           | 1798.19   | J/molxK | 1132.03         | Joback Method |
| cpg           | 1822.07   | J/molxK | 1175.16         | Joback Method |
| cpg           | 1844.36   | J/molxK | 1218.28         | Joback Method |
| cpg           | 1865.21   | J/molxK | 1261.41         | Joback Method |
| dvisc         | 0.0006755 | Paxs    | 488.67          | Joback Method |
| dvisc         | 0.0002218 | Paxs    | 574.33          | Joback Method |

|       |           |      |         |               |
|-------|-----------|------|---------|---------------|
| dvisc | 0.0000973 | Paxs | 660.00  | Joback Method |
| dvisc | 0.0000515 | Paxs | 745.66  | Joback Method |
| dvisc | 0.0000311 | Paxs | 831.33  | Joback Method |
| dvisc | 0.0000207 | Paxs | 917.00  | Joback Method |
| dvisc | 0.0000147 | Paxs | 1002.66 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R528564&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R528564&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>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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