

# Tetradecanoic acid, hexadecyl ester

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Myristic acid, hexadecyl ester<br>Cetyl myristate<br>Hexadecyl tetradecanoate<br>Hexadecylmyristate<br>Schercemol CM |
| <b>Inchi:</b>               | InChI=1S/C30H60O2/c1-3-5-7-9-11-13-15-16-17-19-21-23-25-27-29-32-30(31)28-26-24-                                     |
| <b>InchiKey:</b>            | QAKXLTNAJLFSQC-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C30H60O2   |
| <b>SMILES:</b>              | CCCCCCCCCCCCCCCCOC(=O)CCCCCCCCCCCCCC   |
| <b>Mol. weight [g/mol]:</b> | 452.80   |
| <b>CAS:</b>                 | 2599-01-1  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -32.20  | kJ/mol               | Joback Method  |
| hf            | -907.33 | kJ/mol               | Joback Method  |
| hfus          | 76.24   | kJ/mol               | Joback Method  |
| hvap          | 91.53   | kJ/mol               | Joback Method  |
| log10ws       | -11.24  |                      | Crippen Method |
| logp          | 10.712  |                      | Crippen Method |
| mcvol         | 441.000 | ml/mol               | McGowan Method |
| pc            | 609.06  | kPa                  | Joback Method  |
| rinpol        | 3148.72 |                      | NIST Webbook   |
| rinpol        | 3148.72 |                      | NIST Webbook   |
| tb            | 962.09  | K                    | Joback Method  |
| tc            | 1195.84 | K                    | Joback Method  |
| tf            | 500.02  | K                    | Joback Method  |
| vc            | 1.740   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1548.95 | J/mol×K | 962.09          | Joback Method |
| cpg           | 1575.26 | J/mol×K | 1001.05         | Joback Method |

|       |           |         |         |               |
|-------|-----------|---------|---------|---------------|
| cpg   | 1599.65   | J/molxK | 1040.01 | Joback Method |
| cpg   | 1622.22   | J/molxK | 1078.97 | Joback Method |
| cpg   | 1643.07   | J/molxK | 1117.92 | Joback Method |
| cpg   | 1662.31   | J/molxK | 1156.88 | Joback Method |
| cpg   | 1680.03   | J/molxK | 1195.84 | Joback Method |
| dvisc | 0.0004872 | Paxs    | 500.02  | Joback Method |
| dvisc | 0.0001913 | Paxs    | 577.03  | Joback Method |
| dvisc | 0.0000936 | Paxs    | 654.04  | Joback Method |
| dvisc | 0.0000532 | Paxs    | 731.05  | Joback Method |
| dvisc | 0.0000337 | Paxs    | 808.07  | Joback Method |
| dvisc | 0.0000231 | Paxs    | 885.08  | Joback Method |
| dvisc | 0.0000168 | Paxs    | 962.09  | 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=C2599011&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2599011&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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