

# Tetradecanoic acid

|                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
|----------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 1-Tridecanecarboxylic acid<br>Acide Myristique<br>Crodacid<br>Emery 655<br>Hydrofol acid 1495<br>Hystrene 9014<br>Hystrene 9514<br>Myristic acid<br>Myristic acid (tetradecanoic acid)<br>N-MYRISTIC ACID<br>NSC 5028<br>Neo-Fat 14<br>Philacid 1400<br>Prifac 2942<br>Prifrac 2942<br>Tetradecanoic (Myristic) acid<br>Tetradecanoic acid (=Myristic acid)<br>Tetradecanoic acid (myristic acid)<br>Univol U 316S<br>n-Tetradecan-1-oic acid<br>n-Tetradecanoic acid<br>n-Tetradecoic acid |
| Inchi:               | InChI=1S/C14H28O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14(15)16/h2-13H2,1H3,(H,15,16)                                                                                                                                                                                                                                                                                                                                                                                                             |
| InchiKey:            | TUNFSRHWOTWDNC-UHFFFAOYSA-N                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| Formula:             | C14H28O2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| SMILES:              | CCCCCCCCCCCCC(=O)O                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| Mol. weight [g/mol]: | 228.37                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| CAS:                 | 544-63-8                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |

## Physical Properties

| Property code | Value           | Unit   | Source        |
|---------------|-----------------|--------|---------------|
| chl           | -8676.70 ± 1.40 | kJ/mol | NIST Webbook  |
| chs           | -8675.90 ± 9.60 | kJ/mol | NIST Webbook  |
| gf            | -198.74         | kJ/mol | Joback Method |
| hf            | -597.10         | kJ/mol | Joback Method |

|         |                     |        |                                                                                                                                        |
|---------|---------------------|--------|----------------------------------------------------------------------------------------------------------------------------------------|
| hfus    | 44.75               | kJ/mol | Solid-liquid phase equilibria of (n-octadecane with myristic, and palmitic acid) binary mixtures used as phase change materials (PCMs) |
| hfus    | 43.70               | kJ/mol | Solid-Liquid Equilibrium of Binary Systems Containing Fatty Acids and Fatty Alcohols Using Differential Scanning Calorimetry           |
| hsub    | 169.00 ± 9.00       | kJ/mol | NIST Webbook                                                                                                                           |
| hvap    | 70.18               | kJ/mol | Joback Method                                                                                                                          |
| log10ws | -5.33               |        | Aqueous Solubility Prediction Method                                                                                                   |
| logp    | 4.772               |        | Crippen Method                                                                                                                         |
| mcpvol  | 215.560             | ml/mol | McGowan Method                                                                                                                         |
| pc      | 1644.20 ± 85.00     | kPa    | NIST Webbook                                                                                                                           |
| pt      | 2.13e-05 ± 1.07e-05 | kPa    | NIST Webbook                                                                                                                           |
| rinpol  | 1767.10             |        | NIST Webbook                                                                                                                           |
| rinpol  | 1765.00             |        | NIST Webbook                                                                                                                           |
| rinpol  | 1740.00             |        | NIST Webbook                                                                                                                           |
| rinpol  | 1750.00             |        | NIST Webbook                                                                                                                           |
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| rinpol  | 1765.00             |        | NIST Webbook                                                                                                                           |
| rinpol  | 1787.00             |        | NIST Webbook                                                                                                                           |
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| rinpol  | 1769.70             |        | NIST Webbook                                                                                                                           |
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| ripol | 2724.00       |   | NIST Webbook                                                                                                                                 |
| ripol | 2713.00       |   | NIST Webbook                                                                                                                                 |
| ripol | 2680.00       |   | NIST Webbook                                                                                                                                 |
| tb    | 665.77        | K | Joback Method                                                                                                                                |
| tc    | 765.19 ± 3.00 | K | NIST Webbook                                                                                                                                 |
| tf    | 327.03        | K | Measurement and PC-SAFT modeling of solid-liquid equilibrium of deep eutectic solvents of quaternary ammonium chlorides and carboxylic acids |
| tf    | 327.60        | K | Solid Liquid Equilibria in the Binary Systems of Saturated Fatty Acids or Triglycerides (C12 to C18) + Hexadecane                            |
| tf    | 327.48        | K | Solid-Liquid Equilibrium of Binary Fatty Acid Mixtures                                                                                       |
| tf    | 327.50        | K | Study of the Effect of Pressure on Melting Behavior of Saturated Fatty Acids in Liquid or Supercritical Carbon Dioxide                       |
| tf    | 327.85        | K | Prediction of the properties of eutectic fatty acid phase change materials                                                                   |
| tf    | 327.50        | K | High pressure solid liquid equilibria of fatty acids                                                                                         |
| tf    | 327.82        | K | Aqueous Solubility Prediction Method                                                                                                         |

|    |               |         |                                                                                                                                                                    |
|----|---------------|---------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| tf | 328.88        | K       | The solid liquid phase diagrams of binary mixtures of even saturated fatty acids differing by six carbon atoms                                                     |
| tf | 326.15        | K       | Preparation of paraffin and fatty acid phase changing nanoemulsions for heat transfer                                                                              |
| tf | 329.05        | K       | Solid-liquid phase equilibrium diagrams of binary mixtures containing fatty acids, fatty alcohol compounds and tripalmitin using differential scanning calorimetry |
| tt | 327.05 ± 0.50 | K       | NIST Webbook                                                                                                                                                       |
| tt | 327.32 ± 0.02 | K       | NIST Webbook                                                                                                                                                       |
| vc | 0.845         | m3/kmol | Joback Method                                                                                                                                                      |

# Temperature Dependent Properties

| Property code | Value         | Unit    | Temperature [K] | Source        |
|---------------|---------------|---------|-----------------|---------------|
| cpg           | 676.89        | J/mol×K | 804.44          | Joback Method |
| cpg           | 651.47        | J/mol×K | 748.97          | Joback Method |
| cpg           | 637.85        | J/mol×K | 721.24          | Joback Method |
| cpg           | 623.60        | J/mol×K | 693.50          | Joback Method |
| cpg           | 608.69        | J/mol×K | 665.77          | Joback Method |
| cpg           | 688.73        | J/mol×K | 832.18          | Joback Method |
| cpg           | 664.48        | J/mol×K | 776.71          | Joback Method |
| cps           | 432.01        | J/mol×K | 298.15          | NIST Webbook  |
| cps           | 523.00        | J/mol×K | 298.00          | NIST Webbook  |
| dvisc         | 0.0002574     | Pa×s    | 512.03          | Joback Method |
| dvisc         | 0.0005619     | Pa×s    | 460.78          | Joback Method |
| dvisc         | 0.0000798     | Pa×s    | 614.52          | Joback Method |
| dvisc         | 0.0052331     | Pa×s    | 358.29          | Joback Method |
| dvisc         | 0.0000509     | Pa×s    | 665.77          | Joback Method |
| dvisc         | 0.0001359     | Pa×s    | 563.28          | Joback Method |
| dvisc         | 0.0014913     | Pa×s    | 409.54          | Joback Method |
| hfust         | 36.28         | kJ/mol  | 317.00          | NIST Webbook  |
| hfust         | 45.10         | kJ/mol  | 327.00          | NIST Webbook  |
| hfust         | 45.10         | kJ/mol  | 327.00          | NIST Webbook  |
| hfust         | 45.00         | kJ/mol  | 326.50          | NIST Webbook  |
| hfust         | 40.10         | kJ/mol  | 326.60          | NIST Webbook  |
| hfust         | 45.75         | kJ/mol  | 326.20          | NIST Webbook  |
| hsubt         | 140.00 ± 4.00 | kJ/mol  | 311.85          | NIST Webbook  |

|       |               |        |        |                                                                                                |
|-------|---------------|--------|--------|------------------------------------------------------------------------------------------------|
| hsubt | 139.70 ± 3.80 | kJ/mol | 318.50 | NIST Webbook                                                                                   |
| hvapt | 111.20        | kJ/mol | 298.00 | Vapor Pressures and Vaporization, Sublimation, and Fusion Enthalpies of Some Fatty Acids       |
| hvapt | 100.40        | kJ/mol | 421.00 | NIST Webbook                                                                                   |
| hvapt | 91.60         | kJ/mol | 511.00 | NIST Webbook                                                                                   |
| hvapt | 104.10 ± 2.00 | kJ/mol | 348.50 | NIST Webbook                                                                                   |
| hvapt | 88.90         | kJ/mol | 455.00 | NIST Webbook                                                                                   |
| pvap  | 9.33          | kPa    | 512.60 | Vapor pressure data for fatty acids obtained using an adaptation of the DSC technique          |
| pvap  | 8.00          | kPa    | 508.20 | Vapor pressure data for fatty acids obtained using an adaptation of the DSC technique          |
| pvap  | 6.67          | kPa    | 503.10 | Vapor pressure data for fatty acids obtained using an adaptation of the DSC technique          |
| pvap  | 1.33          | kPa    | 464.60 | Vapor pressure data for fatty acids obtained using an adaptation of the DSC technique          |
| pvap  | 2.67          | kPa    | 480.80 | Vapor pressure data for fatty acids obtained using an adaptation of the DSC technique          |
| pvap  | 5.33          | kPa    | 497.20 | Vapor pressure data for fatty acids obtained using an adaptation of the DSC technique          |
| pvap  | 4.00          | kPa    | 489.50 | Vapor pressure data for fatty acids obtained using an adaptation of the DSC technique          |
| rhoI  | 758.00        | kg/m3  | 473.20 | Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K |

|       |        |         |        |                                                                                                |
|-------|--------|---------|--------|------------------------------------------------------------------------------------------------|
| rhoI  | 769.30 | kg/m3   | 458.20 | Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K |
| rhoI  | 780.90 | kg/m3   | 443.20 | Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K |
| rhoI  | 861.30 | kg/m3   | 332.10 | Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K |
| rhoI  | 791.70 | kg/m3   | 427.90 | Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K |
| rhoI  | 806.70 | kg/m3   | 408.20 | Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K |
| rhoI  | 821.40 | kg/m3   | 388.20 | Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K |
| rhoI  | 835.60 | kg/m3   | 368.20 | Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K |
| rhoI  | 846.90 | kg/m3   | 352.10 | Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K |
| sfust | 114.00 | J/mol×K | 317.00 | NIST Webbook                                                                                   |

# Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 523.20 | K    | 13.30          | NIST Webbook |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.57451e+01                   |
| Coeff. B                    | -5.46750e+03                  |
| Coeff. C                    | -1.07769e+02                  |
| Temperature range (K), min. | 461.48                        |
| Temperature range (K), max. | 631.79                        |

| Information                 | Value                                                  |
|-----------------------------|--------------------------------------------------------|
| Property code               | pvap                                                   |
| Equation                    | $\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$ |
| Coeff. A                    | 2.20853e+02                                            |
| Coeff. B                    | -2.15189e+04                                           |
| Coeff. C                    | -2.86975e+01                                           |
| Coeff. D                    | 9.02023e-06                                            |
| Temperature range (K), min. | 327.55                                                 |
| Temperature range (K), max. | 756.00                                                 |

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## Legend

|          |                                                 |
|----------|-------------------------------------------------|
| chl:     | Standard liquid enthalpy of combustion          |
| chs:     | Standard solid enthalpy of combustion           |
| cpg:     | Ideal gas heat capacity                         |
| cps:     | Solid phase heat capacity                       |
| dvisc:   | Dynamic viscosity                               |
| gf:      | Standard Gibbs free energy of formation         |
| hf:      | Enthalpy of formation at standard conditions    |
| hfus:    | Enthalpy of fusion at standard conditions       |
| hfust:   | Enthalpy of fusion at a given temperature       |
| hsub:    | Enthalpy of sublimation at standard conditions  |
| hsubt:   | Enthalpy of sublimation at a given temperature  |
| hvap:    | Enthalpy of vaporization at standard conditions |
| hvapt:   | Enthalpy of vaporization at a given temperature |
| log10ws: | Log10 of Water solubility in mol/l              |
| logp:    | Octanol/Water partition coefficient             |
| mcvol:   | McGowan's characteristic volume                 |
| pc:      | Critical Pressure                               |
| pt:      | Triple Point Pressure                           |
| pvap:    | Vapor pressure                                  |

|                |                                          |
|----------------|------------------------------------------|
| <b>rho:</b>    | Liquid Density                           |
| <b>rinpol:</b> | Non-polar retention indices              |
| <b>ripol:</b>  | Polar retention indices                  |
| <b>sfust:</b>  | Entropy of fusion at a given temperature |
| <b>tb:</b>     | Normal Boiling Point Temperature         |
| <b>tbrp:</b>   | Boiling point at reduced pressure        |
| <b>tc:</b>     | Critical Temperature                     |
| <b>tf:</b>     | Normal melting (fusion) point            |
| <b>tt:</b>     | Triple Point Temperature                 |
| <b>vc:</b>     | Critical Volume                          |

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