

# E-11-Tetradecenoic acid

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C14H26O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14(15)16/h3-4H,2,5-13H2,1H3,(H, |
| <b>InchiKey:</b>            | FWWOMPFHMRPXIH-ONEGZZNKSA-N  |
| <b>Formula:</b>             | C14H26O2   |
| <b>SMILES:</b>              | CCC=CCCCCCCCC(=O)O   |
| <b>Mol. weight [g/mol]:</b> | 226.35   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -118.52 | kJ/mol               | Joback Method  |
| hf            | -479.88 | kJ/mol               | Joback Method  |
| hfus          | 37.90   | kJ/mol               | Joback Method  |
| hvap          | 70.14   | kJ/mol               | Joback Method  |
| log10ws       | -4.64   |                      | Crippen Method |
| logp          | 4.548   |                      | Crippen Method |
| mcvol         | 211.260 | ml/mol               | McGowan Method |
| pc            | 1803.09 | kPa                  | Joback Method  |
| ripol         | 2537.00 |                      | NIST Webbook   |
| ripol         | 2537.00 |                      | NIST Webbook   |
| tb            | 669.93  | K                    | Joback Method  |
| tc            | 840.79  | K                    | Joback Method  |
| tf            | 353.21  | K                    | Joback Method  |
| vc            | 0.825   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 586.83    | J/molxK | 669.93          | Joback Method |
| cpg           | 601.22    | J/molxK | 698.41          | Joback Method |
| cpg           | 614.96    | J/molxK | 726.88          | Joback Method |
| cpg           | 628.06    | J/molxK | 755.36          | Joback Method |
| cpg           | 640.56    | J/molxK | 783.84          | Joback Method |
| cpg           | 652.48    | J/molxK | 812.32          | Joback Method |
| cpg           | 663.86    | J/molxK | 840.79          | Joback Method |
| dvisc         | 0.0051406 | Paxs    | 353.21          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0013810 | Paxs | 406.00 | Joback Method |
| dvisc | 0.0005020 | Paxs | 458.78 | Joback Method |
| dvisc | 0.0002249 | Paxs | 511.57 | Joback Method |
| dvisc | 0.0001171 | Paxs | 564.36 | Joback Method |
| dvisc | 0.0000681 | Paxs | 617.14 | Joback Method |
| dvisc | 0.0000432 | Paxs | 669.93 | 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=U130962&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U130962&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>ripol:</b>   | 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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