

# 4-Decenoic acid, ethyl ester, (z)-

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Other names:         | Ethyl cis-4-decenoate<br>Ethyl (4Z)-4-decenoate<br>Ethyl (Z)-4-decenoate         |
| Inchi:               | InChI=1S/C12H22O2/c1-3-5-6-7-8-9-10-11-12(13)14-4-2/h8-9H,3-7,10-11H2,1-2H3/b9-8 |
| InchiKey:            | AWNIQMQADACLCJ-HJWRWDBZSA-N                                                      |
| Formula:             | C12H22O2                                                                         |
| SMILES:              | CCCCC/C=C\CCC(=O)OCC                                                             |
| Mol. weight [g/mol]: | 198.31                                                                           |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| af            | 0.5847  |        | Cheméo Relay (1.0) |
| gf            | -103.54 | kJ/mol | Joback Method      |
| hf            | -520.69 | kJ/mol | Cheméo Relay (1.0) |
| hfus          | 29.82   | kJ/mol | Joback Method      |
| hvap          | 67.43   | kJ/mol | Cheméo Relay (1.0) |
| ie            | 8.91    | eV     | Cheméo Relay (1.0) |
| log10ws       | -3.61   |        | Cheméo Relay (1.0) |
| logp          | 3.466   |        | Crippen Method     |
| mcvol         | 183.080 | ml/mol | McGowan Method     |
| pc            | 1937.24 | kPa    | Joback Method      |
| rinpol        | 1345.00 |        | NIST Webbook       |
| rinpol        | 1361.00 |        | NIST Webbook       |
| rinpol        | 1363.00 |        | NIST Webbook       |
| rinpol        | 1345.00 |        | NIST Webbook       |
| rinpol        | 1361.00 |        | NIST Webbook       |
| rinpol        | 1361.00 |        | NIST Webbook       |
| rinpol        | 1359.00 |        | NIST Webbook       |
| rinpol        | 1363.00 |        | NIST Webbook       |
| rinpol        | 1363.00 |        | NIST Webbook       |
| rinpol        | 1363.00 |        | NIST Webbook       |
| rinpol        | 1361.00 |        | NIST Webbook       |
| ripol         | 1699.00 |        | NIST Webbook       |
| ripol         | 1699.00 |        | NIST Webbook       |
| tb            | 495.60  | K      | Cheméo Relay (1.0) |
| tc            | 682.48  | K      | Cheméo Relay (1.0) |
| tf            | 191.36  | K      | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 445.74    | J/mol×K | 554.41          | Joback Method |
| cpg           | 461.06    | J/mol×K | 583.82          | Joback Method |
| cpg           | 475.72    | J/mol×K | 613.24          | Joback Method |
| cpg           | 489.74    | J/mol×K | 642.65          | Joback Method |
| cpg           | 503.13    | J/mol×K | 672.07          | Joback Method |
| cpg           | 515.92    | J/mol×K | 701.48          | Joback Method |
| cpg           | 528.11    | J/mol×K | 730.90          | Joback Method |
| dvisc         | 0.0028734 | Pa×s    | 292.08          | Joback Method |
| dvisc         | 0.0012967 | Pa×s    | 335.80          | Joback Method |
| dvisc         | 0.0007029 | Pa×s    | 379.52          | Joback Method |
| dvisc         | 0.0004324 | Pa×s    | 423.25          | Joback Method |
| dvisc         | 0.0002914 | Pa×s    | 466.97          | Joback Method |
| dvisc         | 0.0002101 | Pa×s    | 510.69          | Joback Method |
| dvisc         | 0.0001595 | Pa×s    | 554.41          | Joback Method |

## Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C7367842&Units=SI>

Joback Method: [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

## Legend

**af:** Acentric Factor

**cpg:** Ideal gas heat capacity

**dvisc:** 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>ie:</b>      | Ionization energy                               |
| <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>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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