

# 4-Ethyl-4-decanolide

|                      |                                                                      |
|----------------------|----------------------------------------------------------------------|
| Inchi:               | InChI=1S/C12H22O2/c1-3-5-6-7-9-12(4-2)10-8-11(13)14-12/h3-10H2,1-2H3 |
| InchiKey:            | ZYGXMFVFBKWHGI-UHFFFAOYSA-N                                          |
| Formula:             | C12H22O2                                                             |
| SMILES:              | CCCCCCC1(CC)CCC(=O)O1                                                |
| Mol. weight [g/mol]: | 198.30                                                               |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -127.49 | kJ/mol  | Joback Method  |
| hf            | -484.99 | kJ/mol  | Joback Method  |
| hfus          | 21.96   | kJ/mol  | Joback Method  |
| hvap          | 50.17   | kJ/mol  | Joback Method  |
| log10ws       | -3.71   |         | Crippen Method |
| logp          | 3.443   |         | Crippen Method |
| mcvol         | 176.520 | ml/mol  | McGowan Method |
| pc            | 2227.09 | kPa     | Joback Method  |
| rinpol        | 1567.00 |         | NIST Webbook   |
| rinpol        | 1567.00 |         | NIST Webbook   |
| ripol         | 2160.00 |         | NIST Webbook   |
| ripol         | 2160.00 |         | NIST Webbook   |
| tb            | 584.25  | K       | Joback Method  |
| tc            | 790.33  | K       | Joback Method  |
| tf            | 354.59  | K       | Joback Method  |
| vc            | 0.674   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 468.27 | J/mol×K | 584.25          | Joback Method |
| cpg           | 486.58 | J/mol×K | 618.60          | Joback Method |
| cpg           | 503.97 | J/mol×K | 652.94          | Joback Method |
| cpg           | 520.54 | J/mol×K | 687.29          | Joback Method |
| cpg           | 536.36 | J/mol×K | 721.64          | Joback Method |
| cpg           | 551.53 | J/mol×K | 755.99          | Joback Method |

## Sources

|                 |                                                                                                                                           |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R434672&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R434672&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <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>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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