

# 2(3H)-Furanone, 3-hexyldihydro-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 3-hexyldihydrofuran-2(3H)-one                                 |
| <b>Inchi:</b>               | InChI=1S/C10H18O2/c1-2-3-4-5-6-9-7-8-12-10(9)11/h9H,2-8H2,1H3 |
| <b>InchiKey:</b>            | IBVDLVUXSDSVQF-UHFFFAOYSA-N                                   |
| <b>Formula:</b>             | C10H18O2  |
| <b>SMILES:</b>              | CCCCCCC1CCOC1=O   |
| <b>Mol. weight [g/mol]:</b> | 170.25  |
| <b>CAS:</b>                 | 18436-37-8  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -138.84 | kJ/mol  | Joback Method  |
| hf            | -458.95 | kJ/mol  | Joback Method  |
| hfus          | 23.08   | kJ/mol  | Joback Method  |
| hvap          | 46.87   | kJ/mol  | Joback Method  |
| log10ws       | -2.52   |         | Crippen Method |
| logp          | 2.520   |         | Crippen Method |
| mcvol         | 148.340 | ml/mol  | McGowan Method |
| pc            | 2571.50 | kPa     | Joback Method  |
| rinpol        | 1441.00 |         | NIST Webbook   |
| tb            | 538.25  | K       | Joback Method  |
| tc            | 742.73  | K       | Joback Method  |
| tf            | 308.15  | K       | Joback Method  |
| vc            | 0.565   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 370.23 | J/molxK | 538.25          | Joback Method |
| cpg           | 387.45 | J/molxK | 572.33          | Joback Method |
| cpg           | 403.86 | J/molxK | 606.41          | Joback Method |
| cpg           | 419.47 | J/molxK | 640.49          | Joback Method |
| cpg           | 434.30 | J/molxK | 674.57          | Joback Method |
| cpg           | 448.34 | J/molxK | 708.65          | Joback Method |
| cpg           | 461.59 | J/molxK | 742.73          | 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=C18436378&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C18436378&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>h vap:</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>r in pol:</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                                 |

Latest version available from:

<https://www.cheméo.com/cid/76-573-2/2-3H-Furanone-3-hexyldihydro.pdf>

Generated by Cheméo on 2024-04-29 08:15:55.785914632 +0000 UTC m=+16667804.706491956.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.