# «delta»-hexadecalactone

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|---|---|
| **Other names:** | Hexadecalactone |
| | 2H-Pyran-2-one, tetrahydro-6-undecyl- |
| | tetrahydro-6-undecyl-2H-pyran-2-one |
| | 6-Undecyltetrahydro-2H-pyran-2-one |
| **Inchi:** | InChI=1S/C16H30O2/c1-2-3-4-5-6-7-8-9-10-12-15-13-11-14-16(17)18-15/h15H,2-14H2,1 |
| **InchiKey:** | ZMJKQSSFLIFELJ-UHFFFAOYSA-N |
| **Formula:** | C16H30O2 |
| **SMILES:** | CCCCCCCCCCCC1CCCC(=O)O1 |
| **Mol. weight [g/mol]:** | 254.41 |
| **CAS:** | 7370-44-7 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -100.42 | kJ/mol | Joback Method |
| hf | -588.95 | kJ/mol | Joback Method |
| hfus | 36.52 | kJ/mol | Joback Method |
| hvap | 60.40 | kJ/mol | Joback Method |
| log10ws | -5.39 | | Crippen Method |
| logp | 5.003 | | Crippen Method |
| mcvol | 232.880 | ml/mol | McGowan Method |
| pc | 1570.96 | kPa | Joback Method |
| rinpol | 2141.90 | | NIST Webbook |
| rinpol | 2154.00 | | NIST Webbook |
| rinpol | 2141.90 | | NIST Webbook |
| rinpol | 2154.00 | | NIST Webbook |
| tb | 679.80 | K | Joback Method |
| tc | 874.67 | K | Joback Method |
| tf | 372.25 | K | Joback Method |
| vc | 0.892 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 690.53 | J/mol×K | 679.80 | Joback Method |

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|---|---|---|---|---|
| cpg | 711.31 | J/mol×K | 712.28 | Joback Method |
| cpg | 730.98 | J/mol×K | 744.76 | Joback Method |
| cpg | 749.56 | J/mol×K | 777.24 | Joback Method |
| cpg | 767.05 | J/mol×K | 809.71 | Joback Method |
| cpg | 783.48 | J/mol×K | 842.19 | Joback Method |
| cpg | 798.85 | J/mol×K | 874.67 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C7370447&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |