# 6-heptadecalactone

**Inchi:** InChI=1S/C16H30O2/c1-2-3-4-5-6-7-8-9-12-15-13-10-11-14-16(17)18-15/h15H,2-14H2,1
**InchiKey:** JDBCCUBGERLOBZ-UHFFFAOYSA-N
**Formula:** C16H30O2
**SMILES:** CCCCCCCCCCC1CCCCC(=O)O1
**Mol. weight [g/mol]:** 254.41

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -112.52 | kJ/mol | Joback Method |
| hf | -595.11 | kJ/mol | Joback Method |
| hfus | 34.42 | kJ/mol | Joback Method |
| hvap | 60.57 | kJ/mol | Joback Method |
| log10ws | -5.39 | | Crippen Method |
| logp | 5.003 | | Crippen Method |
| mcvol | 232.880 | ml/mol | McGowan Method |
| pc | 1602.56 | kPa | Joback Method |
| ripol | 2903.00 | | NIST Webbook |
| ripol | 2903.00 | | NIST Webbook |
| tb | 684.07 | K | Joback Method |
| tc | 884.29 | K | Joback Method |
| tf | 368.73 | K | Joback Method |
| vc | 0.884 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 693.78 | J/mol×K | 684.07 | Joback Method |
| cpg | 715.34 | J/mol×K | 717.44 | Joback Method |
| cpg | 735.70 | J/mol×K | 750.81 | Joback Method |
| cpg | 754.86 | J/mol×K | 784.18 | Joback Method |
| cpg | 772.82 | J/mol×K | 817.55 | Joback Method |
| cpg | 789.59 | J/mol×K | 850.92 | Joback Method |
| cpg | 805.19 | J/mol×K | 884.29 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R320424&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 |

# Legend

| | |
|---|---|
| **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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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