# Cyclododecanone 2,2-dimethylpropanediol-1,3 acetal

**Inchi:** InChI=1S/C17H32O2/c1-16(2)14-18-17(19-15-16)12-10-8-6-4-3-5-7-9-11-13-17/h3-15H2

**InchiKey:** YOBIVFGYEOMIEI-UHFFFAOYSA-N

**Formula:** C17H32O2

**SMILES:** CC1(C)COC2(CCCCCCCCCCC2)OC1

**Mol. weight [g/mol]:** 268.43

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -102.56 | kJ/mol | Joback Method |
| hf | -549.89 | kJ/mol | Joback Method |
| hfus | 16.32 | kJ/mol | Joback Method |
| hvap | 61.87 | kJ/mol | Joback Method |
| log10ws | -5.27 | | Crippen Method |
| logp | 5.060 | | Crippen Method |
| mcvol | 240.410 | ml/mol | McGowan Method |
| pc | 1987.66 | kPa | Joback Method |
| rinpol | 1908.40 | | NIST Webbook |
| rinpol | 1930.30 | | NIST Webbook |
| rinpol | 1896.00 | | NIST Webbook |
| rinpol | 1896.00 | | NIST Webbook |
| ripol | 2307.90 | | NIST Webbook |
| ripol | 2237.90 | | NIST Webbook |
| ripol | 2276.80 | | NIST Webbook |
| ripol | 2237.90 | | NIST Webbook |
| tb | 703.19 | K | Joback Method |
| tc | 964.58 | K | Joback Method |
| tf | 379.45 | K | Joback Method |
| vc | 0.852 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 746.35 | J/mol×K | 703.19 | Joback Method |
| cpg | 776.51 | J/mol×K | 746.75 | Joback Method |

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|---|---|---|---|---|
| cpg | 805.01 | J/mol×K | 790.32 | Joback Method |
| cpg | 832.17 | J/mol×K | 833.88 | Joback Method |
| cpg | 858.32 | J/mol×K | 877.45 | Joback Method |
| cpg | 883.76 | J/mol×K | 921.01 | Joback Method |
| cpg | 908.81 | J/mol×K | 964.58 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R417800&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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |