# Pentanoic acid, 3-(3-hydroxy-5,5-dimethyl-1-oxo-2-cyclohexenyl)-4

**Inchi:** InChI=1S/C13H18O5/c1-7(14)8(4-11(17)18)12-9(15)5-13(2,3)6-10(12)16/h8,15H,4-6H2,1

**InchiKey:** JSHYQFFZRQCDTK-UHFFFAOYSA-N

**Formula:** C13H18O5

**SMILES:** CC(=O)C(CC(=O)O)C1=C(O)CC(C)(C)CC1=O

**Mol. weight [g/mol]:** 254.28

**CAS:** 93647-07-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -568.27 | kJ/mol | Joback Method |
| hf | -879.85 | kJ/mol | Joback Method |
| hfus | 22.77 | kJ/mol | Joback Method |
| hvap | 96.14 | kJ/mol | Joback Method |
| log10ws | -2.01 | | Crippen Method |
| logp | 1.867 | | Crippen Method |
| mcvol | 195.320 | ml/mol | McGowan Method |
| pc | 2899.85 | kPa | Joback Method |
| rinpol | 2040.00 | | NIST Webbook |
| rinpol | 2040.00 | | NIST Webbook |
| tb | 885.23 | K | Joback Method |
| tc | 1097.07 | K | Joback Method |
| tf | 568.07 | K | Joback Method |
| vc | 0.732 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 619.65 | J/mol×K | 885.23 | Joback Method |
| cpg | 632.39 | J/mol×K | 920.54 | Joback Method |
| cpg | 644.83 | J/mol×K | 955.84 | Joback Method |
| cpg | 657.05 | J/mol×K | 991.15 | Joback Method |
| cpg | 669.11 | J/mol×K | 1026.45 | Joback Method |
| cpg | 681.10 | J/mol×K | 1061.76 | Joback Method |
| cpg | 693.09 | J/mol×K | 1097.07 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C93647075&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |