# (3S,3aS,6R,7R,9aS)-6-Hydroxy-1,1,7-trimethyldeca acetate

**Inchi:** InChI=1S/C17H28O3/c1-11(18)20-14-9-15(2,3)12-5-7-16(4)10-17(12,14)8-6-13(16)19/h1
**InchiKey:** BAANKNZYZUSIFA-UHFFFAOYSA-N
**Formula:** C17H28O3
**SMILES:** CC(=O)OC1CC(C)(C)C2CCC3(C)CC12CCC3O
**Mol. weight [g/mol]:** 280.40
**CAS:** 127156-28-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -172.13 | kJ/mol | Joback Method |
| hf | -606.62 | kJ/mol | Joback Method |
| hfus | 19.09 | kJ/mol | Joback Method |
| hvap | 75.15 | kJ/mol | Joback Method |
| log10ws | -4.01 | | Crippen Method |
| logp | 3.296 | | Crippen Method |
| mcvol | 231.120 | ml/mol | McGowan Method |
| pc | 2045.61 | kPa | Joback Method |
| rinpol | 1982.20 | | NIST Webbook |
| rinpol | 1982.20 | | NIST Webbook |
| tb | 776.57 | K | Joback Method |
| tc | 993.74 | K | Joback Method |
| tf | 516.57 | K | Joback Method |
| vc | 0.869 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 767.08 | J/mol×K | 776.57 | Joback Method |
| cpg | 788.49 | J/mol×K | 812.76 | Joback Method |
| cpg | 810.06 | J/mol×K | 848.96 | Joback Method |
| cpg | 832.12 | J/mol×K | 885.15 | Joback Method |
| cpg | 854.99 | J/mol×K | 921.35 | Joback Method |
| cpg | 879.01 | J/mol×K | 957.54 | Joback Method |
| cpg | 904.50 | J/mol×K | 993.74 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C127156289&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

Latest version available from:
https://www.chemeo.com/cid/90-491-7/3S-3aS-6R-7R-9aS-6-Hydroxy-1-1-7-trimethyldecahydro-3a-7-methanocyclop
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