# (3S,8S,9S,10R,13R,14S,17R)-17-((2R,5R)-5-Ethyl-6

**Inchi:** InChI=1S/C30H52O/c1-8-22(20(2)3)10-9-21(4)26-13-14-27-25-12-11-23-19-24(31-7)15-1
**InchiKey:** LOUBEXGURAKLSL-UHFFFAOYSA-N
**Formula:** C30H52O
**SMILES:** CCC(CCC(C)C1CCC2C3CC=C4CC(OC)CCC4(C)C3CCC12C)C(C)C
**Mol. weight [g/mol]:** 428.73
**CAS:** 20194-50-7

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 258.12 | kJ/mol | Joback Method |
| hf | -534.42 | kJ/mol | Joback Method |
| hfus | 37.56 | kJ/mol | Joback Method |
| hvap | 81.86 | kJ/mol | Joback Method |
| log10ws | -8.84 | | Crippen Method |
| logp | 8.679 | | Crippen Method |
| mcvol | 391.690 | ml/mol | McGowan Method |
| pc | 848.01 | kPa | Joback Method |
| rinpol | 3276.90 | | NIST Webbook |
| rinpol | 3276.90 | | NIST Webbook |
| tb | 945.82 | K | Joback Method |
| tc | 1169.34 | K | Joback Method |
| tf | 507.61 | K | Joback Method |
| vc | 1.482 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1467.42 | J/mol×K | 945.82 | Joback Method |
| cpg | 1500.33 | J/mol×K | 983.07 | Joback Method |
| cpg | 1533.39 | J/mol×K | 1020.33 | Joback Method |
| cpg | 1566.94 | J/mol×K | 1057.58 | Joback Method |
| cpg | 1601.27 | J/mol×K | 1094.83 | Joback Method |
| cpg | 1636.72 | J/mol×K | 1132.09 | Joback Method |
| cpg | 1673.61 | J/mol×K | 1169.34 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C20194507&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 |