# Valerenol (trans)

**Inchi:** InChI=1S/C15H24O/c1-10(9-16)8-13-6-4-11(2)14-7-5-12(3)15(13)14/h8,11,13-14,16H,4-
**InchiKey:** KIQXKOUFPHTUQS-CSKARUKUSA-N
**Formula:** C15H24O
**SMILES:** CC(=CC1CCC(C)C2CCC(C)=C12)CO
**Mol. weight [g/mol]:** 220.35
**CAS:** 101628-22-2

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 98.46 | kJ/mol | Joback Method |
| hf | -256.11 | kJ/mol | Joback Method |
| hfus | 29.07 | kJ/mol | Joback Method |
| hvap | 67.35 | kJ/mol | Joback Method |
| log10ws | -4.14 | | Crippen Method |
| logp | 3.698 | | Crippen Method |
| mcvol | 197.760 | ml/mol | McGowan Method |
| pc | 2064.24 | kPa | Joback Method |
| rinpol | 1736.40 | | NIST Webbook |
| rinpol | 1699.00 | | NIST Webbook |
| rinpol | 1736.40 | | NIST Webbook |
| tb | 669.56 | K | Joback Method |
| tc | 870.07 | K | Joback Method |
| tf | 347.47 | K | Joback Method |
| vc | 0.750 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 574.51 | J/mol×K | 669.56 | Joback Method |
| cpg | 592.58 | J/mol×K | 702.98 | Joback Method |
| cpg | 609.62 | J/mol×K | 736.40 | Joback Method |
| cpg | 625.71 | J/mol×K | 769.82 | Joback Method |
| cpg | 640.89 | J/mol×K | 803.24 | Joback Method |
| cpg | 655.23 | J/mol×K | 836.66 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 668.78 | J/mol×K | 870.07 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C101628222&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

| | |
|---|---|
| **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 |