# Valerianol (Khusunol)

**Inchi:** InChI=1S/C15H24O/c1-10-13-5-4-12(9-16)15(13)7-6-11(8-15)14(10,2)3/h11-13,16H,1,4-
**InchiKey:** OOYRHNIVDZZGQV-PWNZVWSESA-N
**Formula:** C15H24O
**SMILES:** C=C1C2CCC(CO)C23CCC(C3)C1(C)C
**Mol. weight [g/mol]:** 220.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 123.33 | kJ/mol | Joback Method |
| hf | -225.04 | kJ/mol | Joback Method |
| hfus | 17.29 | kJ/mol | Joback Method |
| hvap | 62.98 | kJ/mol | Joback Method |
| log10ws | -3.69 | | Crippen Method |
| logp | 3.387 | | Crippen Method |
| mcvol | 191.200 | ml/mol | McGowan Method |
| pc | 2304.74 | kPa | Joback Method |
| rinpol | 1623.00 | | NIST Webbook |
| rinpol | 1626.00 | | NIST Webbook |
| tb | 653.84 | K | Joback Method |
| tc | 861.60 | K | Joback Method |
| tf | 419.41 | K | Joback Method |
| vc | 0.728 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 573.73 | J/mol×K | 653.84 | Joback Method |
| cpg | 592.34 | J/mol×K | 688.47 | Joback Method |
| cpg | 610.14 | J/mol×K | 723.09 | Joback Method |
| cpg | 627.34 | J/mol×K | 757.72 | Joback Method |
| cpg | 644.19 | J/mol×K | 792.34 | Joback Method |
| cpg | 660.92 | J/mol×K | 826.97 | Joback Method |
| cpg | 677.76 | J/mol×K | 861.60 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R613157&Units=SI |

# 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 |