# Drimenal

**Inchi:** InChI=1S/C15H24O/c1-11-6-7-13-14(2,3)8-5-9-15(13,4)12(11)10-16/h6,10,12-13H,5,7-9
**InchiKey:** TUWKAEMGKORGLZ-KCQAQPDRSA-N
**Formula:** C15H24O
**SMILES:** CC1=CCC2C(C)(C)CCCC2(C)C1C=O
**Mol. weight [g/mol]:** 220.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 42.93 | kJ/mol | Joback Method |
| hf | -281.44 | kJ/mol | Joback Method |
| hfus | 15.14 | kJ/mol | Joback Method |
| hvap | 54.25 | kJ/mol | Joback Method |
| log10ws | -4.06 | | Crippen Method |
| logp | 3.984 | | Crippen Method |
| mcvol | 197.760 | ml/mol | McGowan Method |
| pc | 2106.13 | kPa | Joback Method |
| rinpol | 1657.00 | | NIST Webbook |
| ripol | 2045.00 | | NIST Webbook |
| ripol | 2045.00 | | NIST Webbook |
| tb | 617.10 | K | Joback Method |
| tc | 844.17 | K | Joback Method |
| tf | 375.21 | K | Joback Method |
| vc | 0.754 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 548.72 | J/mol×K | 617.10 | Joback Method |
| cpg | 570.40 | J/mol×K | 654.94 | Joback Method |
| cpg | 590.90 | J/mol×K | 692.79 | Joback Method |
| cpg | 610.45 | J/mol×K | 730.63 | Joback Method |
| cpg | 629.30 | J/mol×K | 768.48 | Joback Method |
| cpg | 647.72 | J/mol×K | 806.32 | Joback Method |
| cpg | 665.93 | J/mol×K | 844.17 | Joback Method |

# Sources

| | |
|---|---|
| **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=R440494&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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |