# 1-Penten-3-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-

**Other names:** «beta»-Ionone, methyl-
«beta»-Iraldeine
«beta»-Methylionone
Methyl-«beta»-ionone
5-(2,6,6-Trimethyl-1-cyclohexenyl)-4-penten-3-one
«beta»-N-Methyl ionone
1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)pent-1-en-3-one
1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-1-penten-3-one

**Inchi:** InChI=1S/C14H22O/c1-5-12(15)8-9-13-11(2)7-6-10-14(13,3)4/h8-9H,5-7,10H2,1-4H3/b9

**InchiKey:** LMWNGLDCJDIIBR-CMDGGOBGSA-N

**Formula:** C14H22O

**SMILES:** CCC(=O)C=CC1=C(C)CCCC1(C)C

**Mol. weight [g/mol]:** 206.32

**CAS:** 127-43-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 47.96 | kJ/mol | Joback Method |
| hf | -223.25 | kJ/mol | Joback Method |
| hfus | 19.80 | kJ/mol | Joback Method |
| hvap | 54.36 | kJ/mol | Joback Method |
| log10ws | -4.32 | | Crippen Method |
| logp | 4.048 | | Crippen Method |
| mcvol | 190.230 | ml/mol | McGowan Method |
| pc | 2083.12 | kPa | Joback Method |
| rinpol | 1556.80 | | NIST Webbook |
| ripol | 1988.00 | | NIST Webbook |
| tb | 606.66 | K | Joback Method |
| tc | 821.95 | K | Joback Method |
| tf | 349.47 | K | Joback Method |
| vc | 0.723 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 487.93 | J/mol×K | 606.66 | Joback Method |
| cpg | 506.32 | J/mol×K | 642.54 | Joback Method |
| cpg | 523.69 | J/mol×K | 678.42 | Joback Method |
| cpg | 540.19 | J/mol×K | 714.31 | Joback Method |
| cpg | 555.93 | J/mol×K | 750.19 | Joback Method |
| cpg | 571.04 | J/mol×K | 786.07 | Joback Method |
| cpg | 585.65 | J/mol×K | 821.95 | 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=C127435&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