# 2,3-Dehydro-4-oxo-«beta»-ionol

**Inchi:** InChI=1S/C13H18O2/c1-9(14)5-6-11-10(2)12(15)7-8-13(11,3)4/h5-9,14H,1-4H3/b6-5+
**InchiKey:** FZJGHQBGWXPTDS-AATRIKPKSA-N
**Formula:** C13H18O2
**SMILES:** CC1=C(C=CC(C)O)C(C)(C)C=CC1=O
**Mol. weight [g/mol]:** 206.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -63.43 | kJ/mol | Joback Method |
| hf | -327.46 | kJ/mol | Joback Method |
| hfus | 16.91 | kJ/mol | Joback Method |
| hvap | 66.21 | kJ/mol | Joback Method |
| log10ws | -3.13 | | Crippen Method |
| logp | 2.405 | | Crippen Method |
| mcvol | 177.710 | ml/mol | McGowan Method |
| pc | 2532.82 | kPa | Joback Method |
| ripol | 2800.00 | | NIST Webbook |
| ripol | 2800.00 | | NIST Webbook |
| tb | 688.63 | K | Joback Method |
| tc | 902.66 | K | Joback Method |
| tf | 403.07 | K | Joback Method |
| vc | 0.666 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 486.03 | J/mol×K | 688.63 | Joback Method |
| cpg | 500.81 | J/mol×K | 724.30 | Joback Method |
| cpg | 514.97 | J/mol×K | 759.97 | Joback Method |
| cpg | 528.62 | J/mol×K | 795.65 | Joback Method |
| cpg | 541.83 | J/mol×K | 831.32 | Joback Method |
| cpg | 554.72 | J/mol×K | 866.99 | Joback Method |
| cpg | 567.38 | J/mol×K | 902.66 | 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=U108723&Units=SI |

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