# «alpha»-Elemenone

**Inchi:** InChI=1S/C15H22O/c1-7-15(6)9-14(16)12(10(2)3)8-13(15)11(4)5/h7-8,11H,1,9H2,2-6H3
**InchiKey:** UYBFSLXEYFGANT-OAHLLOKOSA-N
**Formula:** C15H22O
**SMILES:** C=CC1(C)CC(=O)C(=C(C)C)C=C1C(C)C
**Mol. weight [g/mol]:** 218.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 114.43 | kJ/mol | Joback Method |
| hf | -188.37 | kJ/mol | Joback Method |
| hfus | 14.70 | kJ/mol | Joback Method |
| hvap | 53.27 | kJ/mol | Joback Method |
| log10ws | -4.35 | | Crippen Method |
| logp | 4.070 | | Crippen Method |
| mcvol | 200.020 | ml/mol | McGowan Method |
| pc | 1944.08 | kPa | Joback Method |
| rinpol | 1670.00 | | NIST Webbook |
| rinpol | 1670.00 | | NIST Webbook |
| rinpol | 1670.00 | | NIST Webbook |
| tb | 637.11 | K | Joback Method |
| tc | 863.01 | K | Joback Method |
| tf | 351.23 | K | Joback Method |
| vc | 0.758 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 529.15 | J/mol×K | 637.11 | Joback Method |
| cpg | 548.65 | J/mol×K | 674.76 | Joback Method |
| cpg | 567.15 | J/mol×K | 712.41 | Joback Method |
| cpg | 584.79 | J/mol×K | 750.06 | Joback Method |
| cpg | 601.66 | J/mol×K | 787.71 | Joback Method |
| cpg | 617.90 | J/mol×K | 825.36 | Joback Method |
| cpg | 633.61 | J/mol×K | 863.01 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R324491&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 |

# 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 |