# (E)-5,6-Epoxy-«beta»-ionone

**Other names:** trans- «beta»-Ionone epoxide
(E)-4-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]-heptan-1-yl)but-3-en-2-one
**Inchi:** InChI=1S/C13H20O2/c1-10(14)6-9-13-11(2,3)7-5-8-12(13,4)15-13/h6,9H,5,7-8H2,1-4H3/
**InchiKey:** ZTJZJYUGOJYHCU-RMKNXTFCSA-N
**Formula:** C13H20O2
**SMILES:** CC(=O)C=CC12OC1(C)CCCC2(C)C
**Mol. weight [g/mol]:** 208.30

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hfus | 15.55 | kJ/mol | Joback Method |
| logp | 2.869 | | Crippen Method |
| mcvol | 175.450 | ml/mol | McGowan Method |
| rinpol | 1473.00 | | NIST Webbook |
| rinpol | 1441.00 | | NIST Webbook |
| rinpol | 1479.00 | | NIST Webbook |
| ripol | 1995.00 | | NIST Webbook |
| ripol | 2009.00 | | NIST Webbook |
| ripol | 2015.00 | | NIST Webbook |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 470.73 | J/mol×K | 595.62 | Joback Method |
| cpg | 488.22 | J/mol×K | 634.08 | Joback Method |
| cpg | 504.61 | J/mol×K | 672.54 | Joback Method |
| cpg | 520.30 | J/mol×K | 710.99 | Joback Method |
| cpg | 535.71 | J/mol×K | 749.45 | Joback Method |
| cpg | 551.26 | J/mol×K | 787.91 | Joback Method |
| cpg | 567.34 | J/mol×K | 826.37 | Joback Method |

# Sources

| | |
|---|---|
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R407155&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |