# 2(3H)-Benzofuranone, 6-ethenylhexahydro-6-methyl-3-methylene-7-(1-m [3aS-(3a«alpha»,6«alpha»,7«beta»,7a«beta»)]-

**Other names:** 2(3H)-Benzofuranone, 6«alpha»-ethenylhexahydro-6«alpha»-isopropenyl-7«alpha»-methyl-3-methyl
Saussurea lactone, dehydro-
(+)-
Dehydrosaussurea lactone

**Inchi:** InChI=1S/C15H20O2/c1-6-15(5)8-7-11-10(4)14(16)17-13(11)12(15)9(2)3/h6,11-13H,1-2,

**InchiKey:** ZNTHTBBAGNVESR-UHFFFAOYSA-N

**Formula:** C15H20O2

**SMILES:** C=CC1(C)CCC2C(=C)C(=O)OC2C1C(=C)C

**Mol. weight [g/mol]:** 232.32

**CAS:** 28290-35-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 151.21 | kJ/mol | Joback Method |
| hf | -195.64 | kJ/mol | Joback Method |
| hfus | 22.88 | kJ/mol | Joback Method |
| hvap | 55.21 | kJ/mol | Joback Method |
| log10ws | -3.70 | | Crippen Method |
| logp | 3.263 | | Crippen Method |
| mcvol | 195.030 | ml/mol | McGowan Method |
| pc | 2047.46 | kPa | Joback Method |
| rinpol | 1838.40 | | NIST Webbook |
| rinpol | 1838.40 | | NIST Webbook |
| tb | 646.96 | K | Joback Method |
| tc | 877.83 | K | Joback Method |
| tf | 390.54 | K | Joback Method |
| vc | 0.737 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 550.04 | J/mol×K | 646.96 | Joback Method |
| cpg | 570.55 | J/mol×K | 685.44 | Joback Method |
| cpg | 589.93 | J/mol×K | 723.92 | Joback Method |
| cpg | 608.32 | J/mol×K | 762.39 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 625.84 | J/mol×K | 800.87 | Joback Method |
| cpg | 642.65 | J/mol×K | 839.35 | Joback Method |
| cpg | 658.87 | J/mol×K | 877.83 | Joback Method |

# Sources

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|---|---|
| **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=C28290359&Units=SI |
| **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 |
| **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 |