# 3-Isobutenyl-5-methyl-5-vinylbutyrolactone

**Inchi:** InChI=1S/C11H16O2/c1-5-11(4)7-9(6-8(2)3)10(12)13-11/h5-6,9H,1,7H2,2-4H3
**InchiKey:** XWGYDDYYOWAEQP-UHFFFAOYSA-N
**Formula:** C11H16O2
**SMILES:** C=CC1(C)CC(C=C(C)C)C(=O)O1
**Mol. weight [g/mol]:** 180.24

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 15.89 | kJ/mol | Joback Method |
| hf | -251.83 | kJ/mol | Joback Method |
| hfus | 18.05 | kJ/mol | Joback Method |
| hvap | 47.00 | kJ/mol | Joback Method |
| log10ws | -2.76 | | Crippen Method |
| logp | 2.460 | | Crippen Method |
| mcvol | 153.830 | ml/mol | McGowan Method |
| pc | 2611.07 | kPa | Joback Method |
| rinpol | 1324.00 | | NIST Webbook |
| tb | 557.42 | K | Joback Method |
| tc | 785.09 | K | Joback Method |
| tf | 318.28 | K | Joback Method |
| vc | 0.580 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 380.33 | J/mol×K | 557.42 | Joback Method |
| cpg | 397.77 | J/mol×K | 595.36 | Joback Method |
| cpg | 414.17 | J/mol×K | 633.31 | Joback Method |
| cpg | 429.65 | J/mol×K | 671.25 | Joback Method |
| cpg | 444.32 | J/mol×K | 709.20 | Joback Method |
| cpg | 458.33 | J/mol×K | 747.14 | Joback Method |
| cpg | 471.77 | J/mol×K | 785.09 | 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=R229148&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |