# Dehydrofukinone

**Inchi:** InChI=1S/C15H22O/c1-10(2)13-9-15(4)11(3)6-5-7-12(15)8-14(13)16/h8,11H,5-7,9H2,1-4
**InchiKey:** DZOKWSREAZGFFC-ABAIWWIYSA-N
**Formula:** C15H22O
**SMILES:** CC(C)=C1CC2(C)C(=CC1=O)CCCC2C
**Mol. weight [g/mol]:** 218.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 77.68 | kJ/mol | Joback Method |
| hf | -241.88 | kJ/mol | Joback Method |
| hfus | 15.53 | kJ/mol | Joback Method |
| hvap | 54.42 | kJ/mol | Joback Method |
| log10ws | -4.39 | | Crippen Method |
| logp | 4.048 | | Crippen Method |
| mcvol | 193.460 | ml/mol | McGowan Method |
| pc | 2137.41 | kPa | Joback Method |
| rinpol | 1772.00 | | NIST Webbook |
| rinpol | 1772.00 | | NIST Webbook |
| rinpol | 1772.00 | | NIST Webbook |
| rinpol | 1772.00 | | NIST Webbook |
| tb | 651.88 | K | Joback Method |
| tc | 891.67 | K | Joback Method |
| tf | 382.41 | K | Joback Method |
| vc | 0.733 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 539.30 | J/mol×K | 651.88 | Joback Method |
| cpg | 560.66 | J/mol×K | 691.85 | Joback Method |
| cpg | 580.83 | J/mol×K | 731.81 | Joback Method |
| cpg | 599.99 | J/mol×K | 771.78 | Joback Method |
| cpg | 618.29 | J/mol×K | 811.74 | Joback Method |
| cpg | 635.88 | J/mol×K | 851.71 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 652.93 | J/mol×K | 891.67 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R162882&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 |