# Caryophylla-3(15),7(14)-dien-6-one

**Inchi:** InChI=1S/C15H22O/c1-10-5-7-13-12(9-15(13,3)4)11(2)14(16)8-6-10/h12-13H,1-2,5-9H2,
**InchiKey:** NZPOBSKADKAQSR-UHFFFAOYSA-N
**Formula:** C15H22O
**SMILES:** C=C1CCC(=O)C(=C)C2CC(C)(C)C2CC1
**Mol. weight [g/mol]:** 218.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 106.79 | kJ/mol | Joback Method |
| hf | -212.45 | kJ/mol | Joback Method |
| hfus | 12.34 | kJ/mol | Joback Method |
| hvap | 52.78 | kJ/mol | Joback Method |
| log10ws | -4.15 | | Crippen Method |
| logp | 3.904 | | Crippen Method |
| mcvol | 193.460 | ml/mol | McGowan Method |
| pc | 2088.84 | kPa | Joback Method |
| rinpol | 1563.00 | | NIST Webbook |
| tb | 639.14 | K | Joback Method |
| tc | 876.58 | K | Joback Method |
| tf | 392.33 | K | Joback Method |
| vc | 0.722 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 541.15 | J/mol×K | 639.14 | Joback Method |
| cpg | 563.82 | J/mol×K | 678.71 | Joback Method |
| cpg | 585.20 | J/mol×K | 718.29 | Joback Method |
| cpg | 605.43 | J/mol×K | 757.86 | Joback Method |
| cpg | 624.62 | J/mol×K | 797.43 | Joback Method |
| cpg | 642.88 | J/mol×K | 837.00 | Joback Method |
| cpg | 660.33 | J/mol×K | 876.58 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R231200&Units=SI |

# 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 |

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