# «beta»-Atlantone

**Inchi:** InChI=1S/C15H20O/c1-11(2)9-15(16)10-13(4)14-7-5-12(3)6-8-14/h5,7,9H,4,6,8,10H2,1-3
**InchiKey:** RJTSSXMBQPILHQ-UHFFFAOYSA-N
**Formula:** C15H20O
**SMILES:** C=C(CC(=O)C=C(C)C)C1=CC=C(C)CC1
**Mol. weight [g/mol]:** 216.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 170.28 | kJ/mol | Joback Method |
| hf | -75.16 | kJ/mol | Joback Method |
| hfus | 24.94 | kJ/mol | Joback Method |
| hvap | 57.82 | kJ/mol | Joback Method |
| log10ws | -4.69 | | Crippen Method |
| logp | 4.135 | | Crippen Method |
| mcvol | 195.720 | ml/mol | McGowan Method |
| pc | 2045.61 | kPa | Joback Method |
| rinpol | 1670.00 | | NIST Webbook |
| tb | 629.57 | K | Joback Method |
| tc | 846.73 | K | Joback Method |
| tf | 312.16 | K | Joback Method |
| vc | 0.750 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 496.74 | J/mol×K | 629.57 | Joback Method |
| cpg | 514.21 | J/mol×K | 665.76 | Joback Method |
| cpg | 530.60 | J/mol×K | 701.96 | Joback Method |
| cpg | 545.96 | J/mol×K | 738.15 | Joback Method |
| cpg | 560.36 | J/mol×K | 774.35 | Joback Method |
| cpg | 573.85 | J/mol×K | 810.54 | Joback Method |
| cpg | 586.51 | J/mol×K | 846.73 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R504855&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |