# Bicyclo[3.3.1]nona-3,7-diene-2,6-dione

**Inchi:** InChI=1S/C9H8O2/c10-8-3-1-6-5-7(8)2-4-9(6)11/h1-4,6-7H,5H2
**InchiKey:** FEKKORHLKPVNDZ-UHFFFAOYSA-N
**Formula:** C9H8O2
**SMILES:** O=C1C=CC2CC1C=CC2=O
**Mol. weight [g/mol]:** 148.16
**CAS:** 133960-97-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -75.16 | kJ/mol | Joback Method |
| hf | -261.81 | kJ/mol | Joback Method |
| hfus | 10.50 | kJ/mol | Joback Method |
| hvap | 45.05 | kJ/mol | Joback Method |
| ie | 9.45 | eV | NIST Webbook |
| log10ws | -1.16 | | Crippen Method |
| logp | 0.887 | | Crippen Method |
| mcvol | 110.490 | ml/mol | McGowan Method |
| pc | 3881.95 | kPa | Joback Method |
| tb | 565.57 | K | Joback Method |
| tc | 821.71 | K | Joback Method |
| tf | 354.47 | K | Joback Method |
| vc | 0.415 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 270.26 | J/mol×K | 565.57 | Joback Method |
| cpg | 286.15 | J/mol×K | 608.26 | Joback Method |
| cpg | 301.04 | J/mol×K | 650.95 | Joback Method |
| cpg | 314.91 | J/mol×K | 693.64 | Joback Method |
| cpg | 327.75 | J/mol×K | 736.33 | Joback Method |
| cpg | 339.58 | J/mol×K | 779.02 | Joback Method |
| cpg | 350.37 | J/mol×K | 821.71 | 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=C133960971&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 |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |