# 7-Oxabicyclo[2.2.1]heptane-2,5-dione, 3,6-dimethylidene-

**Inchi:** InChI=1S/C8H6O3/c1-3-5(9)8-4(2)6(10)7(3)11-8/h7-8H,1-2H2
**InchiKey:** YIHLCAOATGPYBG-UHFFFAOYSA-N
**Formula:** C8H6O3
**SMILES:** C=C1C(=O)C2OC1C(=O)C2=C
**Mol. weight [g/mol]:** 150.13
**CAS:** 127750-98-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -99.26 | kJ/mol | Joback Method |
| hf | -307.93 | kJ/mol | Joback Method |
| hfus | 15.33 | kJ/mol | Joback Method |
| hvap | 46.72 | kJ/mol | Joback Method |
| ie | 9.40 | eV | NIST Webbook |
| ie | 9.10 | eV | NIST Webbook |
| log10ws | -0.54 | | Crippen Method |
| logp | 0.018 | | Crippen Method |
| mcvol | 102.270 | ml/mol | McGowan Method |
| pc | 3896.50 | kPa | Joback Method |
| tb | 561.10 | K | Joback Method |
| tc | 800.43 | K | Joback Method |
| tf | 402.65 | K | Joback Method |
| vc | 0.393 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 250.41 | J/mol×K | 561.10 | Joback Method |
| cpg | 262.49 | J/mol×K | 600.99 | Joback Method |
| cpg | 273.95 | J/mol×K | 640.88 | Joback Method |
| cpg | 284.80 | J/mol×K | 680.76 | Joback Method |
| cpg | 295.00 | J/mol×K | 720.65 | Joback Method |
| cpg | 304.55 | J/mol×K | 760.54 | Joback Method |
| cpg | 313.43 | J/mol×K | 800.43 | 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=C127750985&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 |
| **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 |