# 4,7-Ethanoisobenzofuran-1,3-dione, 3a,4,7,7a-tetrahydro-, (3a«alpha»,4«alpha»,7«alpha»,7a«alpha»)-

| | |
|---|---|
| **Other names:** | Bicyclo[2.2.2]oct-5-ene-2,3-dicarboxylic anhydride, cis-endo-<br>endo-Bicyclo[2.2.2]octenedicarboxcyclic acid anhydride<br>Bicyclo[2.2.2]oct-5-ene-2,3-dicarboxylic anhydride, endo-<br>Bicyclo[2.2.2]octene-2,3-endo-dicarboxylic anhydride<br>endo-Bicyclo[2.2.2]oct-5-ene-2,3-dicarboxylic anhydride<br>Bicyclo[3.2.1]-5-octene-2,3-dicarboxylic anhydride<br>endo-Bicyclo[2.2.2]-5-octene-2,3-dicarboxylic anhydride<br>Bicyclo[2,2,2]oct-5-ene-2,3-dicarboxylic anhydride, endo- |
| **Inchi:** | InChI=1S/C10H10O3/c11-9-7-5-1-2-6(4-3-5)8(7)10(12)13-9/h1-2,5-8H,3-4H2/t5?,6?,7-,8- |
| **InchiKey:** | YIHKILSPWGDWPR-HYNHDVCUSA-N |
| **Formula:** | C10H10O3 |
| **SMILES:** | O=C1OC(=O)C2C3C=CC(CC3)C12 |
| **Mol. weight [g/mol]:** | 178.18 |
| **CAS:** | 24327-08-0 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -117.68 | kJ/mol | Joback Method |
| hf | -413.61 | kJ/mol | Joback Method |
| hfus | 21.15 | kJ/mol | Joback Method |
| hvap | 50.92 | kJ/mol | Joback Method |
| log10ws | -1.22 | | Crippen Method |
| logp | 0.898 | | Crippen Method |
| mcvol | 123.890 | ml/mol | McGowan Method |
| pc | 3568.53 | kPa | Joback Method |
| tb | 614.04 | K | Joback Method |
| tc | 867.97 | K | Joback Method |
| tf | 408.77 | K | Joback Method |
| tt | 419.20 ± 1.50 | K | NIST Webbook |
| vc | 0.470 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| cpg | 429.62 | J/mol×K | 825.65 | Joback Method |
| cpg | 354.29 | J/mol×K | 614.04 | Joback Method |
| cpg | 371.76 | J/mol×K | 656.36 | Joback Method |
| cpg | 387.98 | J/mol×K | 698.68 | Joback Method |
| cpg | 403.01 | J/mol×K | 741.01 | Joback Method |
| cpg | 416.88 | J/mol×K | 783.33 | Joback Method |
| cpg | 441.28 | J/mol×K | 867.97 | Joback Method |
| hfust | 4.54 | kJ/mol | 419.20 | NIST Webbook |

# 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=C24327080&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
**hfust:** Enthalpy of fusion at a given temperature
**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
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**tt:** Triple Point Temperature
**vc:** Critical Volume