# 4H-1-Benzopyran-4-one

| | |
|---|---|
| **Other names:** | Chromone |
| | Benzo-«gamma»-pyrone |
| | 4H-benzo[b]pyran-4-one |
| **Inchi:** | InChI=1S/C9H6O2/c10-8-5-6-11-9-4-2-1-3-7(8)9/h1-6H |
| **InchiKey:** | OTAFHZMPRISVEM-UHFFFAOYSA-N |
| **Formula:** | C9H6O2 |
| **SMILES:** | O=c1ccoc2ccccc12 |
| **Mol. weight [g/mol]:** | 146.14 |
| **CAS:** | 491-38-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -4169.30 ± 2.90 | kJ/mol | NIST Webbook |
| hf | -148.50 ± 2.90 | kJ/mol | NIST Webbook |
| hfs | -229.80 ± 2.90 | kJ/mol | NIST Webbook |
| hsub | 86.50 ± 1.10 | kJ/mol | NIST Webbook |
| hsub | 81.29 ± 0.16 | kJ/mol | NIST Webbook |
| hsub | 81.30 | kJ/mol | NIST Webbook |
| hsub | 81.30 ± 0.20 | kJ/mol | NIST Webbook |
| log10ws | -6.43 | | Crippen Method |
| logp | 1.793 | | Crippen Method |
| mcvol | 106.190 | ml/mol | McGowan Method |
| tt | 330.27 ± 0.04 | K | NIST Webbook |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cps | 176.80 | J/mol×K | 298.15 | NIST Webbook |
| hfust | 17.31 | kJ/mol | 330.27 | NIST Webbook |
| hfust | 15.44 | kJ/mol | 329.90 | NIST Webbook |
| hfust | 17.31 | kJ/mol | 330.30 | NIST Webbook |
| hvapt | 81.29 | kJ/mol | 298.15 | NIST Webbook |

# Sources

| | |
|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C491383&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **cps:** | Solid phase heat capacity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfs:** | Solid phase enthalpy of formation at standard conditions |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hsub:** | Enthalpy of sublimation at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **tt:** | Triple Point Temperature |