# 2-ACETYL-1,3-CYCLOHEXANEDIONE

**Other names:** 1,3-Cyclohexanedione, 2-acetyl-
**Inchi:** InChI=1S/C8H10O3/c1-5(9)8-6(10)3-2-4-7(8)11/h8H,2-4H2,1H3
**InchiKey:** CHNXDYRMRBQOEF-UHFFFAOYSA-N
**Formula:** C8H10O3
**SMILES:** CC(=O)C1C(=O)CCCC1=O
**Mol. weight [g/mol]:** 154.17

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hfus | 8.93 | kJ/mol | Joback Method |
| ie | 9.09 | eV | Cheméo Relay (1.0) |
| logp | 0.514 | | Crippen Method |
| mcvol | 117.430 | ml/mol | McGowan Method |
| tb | 520.96 | K | Cheméo Relay (1.0) |
| tf | 303.50 ± 1.50 | K | NIST Webbook |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 294.32 | J/mol×K | 591.50 | Joback Method |
| cpg | 309.84 | J/mol×K | 632.36 | Joback Method |
| cpg | 324.52 | J/mol×K | 673.22 | Joback Method |
| cpg | 338.28 | J/mol×K | 714.08 | Joback Method |
| cpg | 351.09 | J/mol×K | 754.94 | Joback Method |
| cpg | 362.87 | J/mol×K | 795.80 | Joback Method |
| cpg | 373.57 | J/mol×K | 836.66 | Joback Method |

## Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 399.70 | K | 2.90 | NIST Webbook |

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|---|---|---|---|---|
| tbrp | 399.50 ± 0.50 | K | 2.90 | NIST Webbook |

# Sources

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|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C4056739&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **ie:** | Ionization energy |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tf:** | Normal melting (fusion) point |