# Methylene diacetate

**Inchi:** InChI=1S/C5H8O4/c1-4(6)8-3-9-5(2)7/h3H2,1-2H3
**InchiKey:** BPGDAMSIGCZZLK-UHFFFAOYSA-N
**Formula:** C5H8O4
**SMILES:** CC(=O)OCOC(C)=O
**Mol. weight [g/mol]:** 132.11
**CAS:** 628-51-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -2273.83 ± 0.91 | kJ/mol | NIST Webbook |
| gf | -476.62 | kJ/mol | Joback Method |
| hf | -780.66 ± 0.93 | kJ/mol | NIST Webbook |
| hfl | -837.04 ± 0.91 | kJ/mol | NIST Webbook |
| hfus | 14.28 | kJ/mol | Joback Method |
| hvap | 56.38 ± 0.25 | kJ/mol | NIST Webbook |
| hvap | 56.40 | kJ/mol | NIST Webbook |
| log10ws | -0.14 | | Crippen Method |
| logp | 0.070 | | Crippen Method |
| mcvol | 96.190 | ml/mol | McGowan Method |
| pc | 3877.12 | kPa | Joback Method |
| rinpol | 782.00 | | NIST Webbook |
| rinpol | 782.00 | | NIST Webbook |
| rinpol | 785.00 | | NIST Webbook |
| tb | 466.38 | K | Joback Method |
| tc | 656.26 | K | Joback Method |
| tf | 290.43 | K | Joback Method |
| vc | 0.363 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 196.70 | J/mol×K | 466.38 | Joback Method |
| cpg | 204.67 | J/mol×K | 498.03 | Joback Method |
| cpg | 212.42 | J/mol×K | 529.67 | Joback Method |

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|---|---|---|---|---|
| cpg | 219.95 | J/mol×K | 561.32 | Joback Method |
| cpg | 227.23 | J/mol×K | 592.97 | Joback Method |
| cpg | 234.25 | J/mol×K | 624.62 | Joback Method |
| cpg | 240.99 | J/mol×K | 656.26 | Joback Method |
| dvisc | 0.0020268 | Pa×s | 290.43 | Joback Method |
| dvisc | 0.0012551 | Pa×s | 319.75 | Joback Method |
| dvisc | 0.0008423 | Pa×s | 349.08 | Joback Method |
| dvisc | 0.0006014 | Pa×s | 378.40 | Joback Method |
| dvisc | 0.0004507 | Pa×s | 407.73 | Joback Method |
| dvisc | 0.0003511 | Pa×s | 437.06 | Joback Method |
| dvisc | 0.0002822 | Pa×s | 466.38 | Joback Method |
| hvapt | 50.60 | kJ/mol | 388.50 | NIST Webbook |

# Sources

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|---|---|
| **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=C628513&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

| | |
|---|---|
| **chl:** | Standard liquid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfl:** | Liquid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization 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 |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |

| | |
|---|---|
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |