

CH₃C(O)OCH(CH₃)C(O)CH₃

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|-----------------------------|--|
| Other names: | 2-Acetoxy-3-butanone 3-acetoxy-2-butanone 2-Butanon-3-ol, acetate 3-(acetyloxy)-2-butanone 2-Ketobutan-3-yl acetate 3-oxo-2-butyl acetate 2-Butanone, 3-(acetyloxy)- Acetoin Acetate 3-oxobutan-2-yl acetate |
| Inchi: | InChI=1S/C6H10O3/c1-4(7)5(2)9-6(3)8/h5H,1-3H3 |
| InchiKey: | ZKPTYCJWRHHBOW-UHFFFAOYSA-N |
| Formula: | C6H10O3 |
| SMILES: | CC(=O)OC(C)C(C)=O |
| Mol. weight [g/mol]: | 130.14 |
| CAS: | 4906-24-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| gf | -365.64 | kJ/mol | Joback Method |
| hf | -529.83 | kJ/mol | Joback Method |
| hfus | 12.16 | kJ/mol | Joback Method |
| hvap | 44.46 | kJ/mol | Joback Method |
| log10ws | -0.59 | | Crippen Method |
| logp | 0.527 | | Crippen Method |
| mcvol | 104.410 | ml/mol | McGowan Method |
| pc | 3555.77 | kPa | Joback Method |
| rinpol | 852.00 | | NIST Webbook |
| rinpol | 856.00 | | NIST Webbook |
| rinpol | 855.00 | | NIST Webbook |
| rinpol | 888.00 | | NIST Webbook |
| rinpol | 888.00 | | NIST Webbook |
| rinpol | 856.00 | | NIST Webbook |
| ripol | 1378.00 | | NIST Webbook |
| ripol | 1358.00 | | NIST Webbook |
| ripol | 1377.00 | | NIST Webbook |
| ripol | 1389.00 | | NIST Webbook |
| ripol | 1389.00 | | NIST Webbook |

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|-------|---------|----------------------|---------------|
| ripol | 1361.00 | | NIST Webbook |
| tb | 466.40 | K | Joback Method |
| tc | 659.46 | K | Joback Method |
| tf | 264.47 | K | Joback Method |
| vc | 0.396 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 215.20 | J/molxK | 466.40 | Joback Method |
| cpg | 224.83 | J/molxK | 498.58 | Joback Method |
| cpg | 234.10 | J/molxK | 530.75 | Joback Method |
| cpg | 243.00 | J/molxK | 562.93 | Joback Method |
| cpg | 251.53 | J/molxK | 595.11 | Joback Method |
| cpg | 259.68 | J/molxK | 627.28 | Joback Method |
| cpg | 267.46 | J/molxK | 659.46 | Joback Method |
| dvisc | 0.0036503 | Paxs | 264.47 | Joback Method |
| dvisc | 0.0019016 | Paxs | 298.12 | Joback Method |
| dvisc | 0.0011308 | Paxs | 331.78 | Joback Method |
| dvisc | 0.0007400 | Paxs | 365.44 | Joback Method |
| dvisc | 0.0005201 | Paxs | 399.09 | Joback Method |
| dvisc | 0.0003862 | Paxs | 432.75 | Joback Method |
| dvisc | 0.0002994 | Paxs | 466.40 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=C4906245&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|---------------|-------------------------|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |

| | |
|------------------|---|
| 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 |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpolar: | Non-polar retention indices |
| ripolar: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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