# 2-Acetoxyisobutyryl chloride

**Other names:** Propanoyl chloride, 2-(acetyloxy)-2-methyl-
2-Chloro-1,1-dimethyl-2-oxoethyl acetate
1-Chlorocarbonyl-1-methylethyl acetate
Acetic acid 2-chloro-1,1-dimethyl-2-oxoethyl ester
Lactoyl chloride, 2-methyl-, acetate
2-acetoxyisobutyroyl chloride
**Inchi:** InChI=1S/C6H9ClO3/c1-4(8)10-6(2,3)5(7)9/h1-3H3
**InchiKey:** RBTCRFLJLUNCLL-UHFFFAOYSA-N
**Formula:** C6H9ClO3
**SMILES:** CC(=O)OC(C)(C)C(=O)Cl
**Mol. weight [g/mol]:** 164.59
**CAS:** 40635-66-3

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -372.29 | kJ/mol | Joback Method |
| hf | -549.04 | kJ/mol | Joback Method |
| hfus | 12.46 | kJ/mol | Joback Method |
| hvap | 47.94 | kJ/mol | Joback Method |
| log10ws | -1.24 | | Crippen Method |
| logp | 1.094 | | Crippen Method |
| mcvol | 116.650 | ml/mol | McGowan Method |
| pc | 3448.03 | kPa | Joback Method |
| tb | 501.04 | K | Joback Method |
| tc | 707.91 | K | Joback Method |
| tf | 311.81 | K | Joback Method |
| vc | 0.440 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 241.93 | J/mol×K | 501.04 | Joback Method |
| cpg | 285.29 | J/mol×K | 673.43 | Joback Method |
| cpg | 277.68 | J/mol×K | 638.95 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 269.55 | J/mol×K | 604.47 | Joback Method |
| cpg | 260.90 | J/mol×K | 570.00 | Joback Method |
| cpg | 251.69 | J/mol×K | 535.52 | Joback Method |
| cpg | 292.41 | J/mol×K | 707.91 | Joback Method |
| dvisc | 0.0003181 | Pa×s | 501.04 | Joback Method |
| dvisc | 0.0004105 | Pa×s | 469.50 | Joback Method |
| dvisc | 0.0005496 | Pa×s | 437.96 | Joback Method |
| dvisc | 0.0007698 | Pa×s | 406.42 | Joback Method |
| dvisc | 0.0011411 | Pa×s | 374.89 | Joback Method |
| dvisc | 0.0018184 | Pa×s | 343.35 | Joback Method |
| dvisc | 0.0031842 | Pa×s | 311.81 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 328.50 ± 0.50 | K | 0.80 | NIST Webbook |

# Sources

**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=C40635663&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |