# Acetic acid, tribromo, 2-methylpropyl ester

**Inchi:** InChI=1S/C6H9Br3O2/c1-4(2)3-11-5(10)6(7,8)9/h4H,3H2,1-2H3
**InchiKey:** GBRCAOJHYDQGKG-UHFFFAOYSA-N
**Formula:** C6H9Br3O2
**SMILES:** CC(C)COC(=O)C(Br)(Br)Br
**Mol. weight [g/mol]:** 352.85

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -190.92 | kJ/mol | Joback Method |
| hf | -347.01 | kJ/mol | Joback Method |
| hfus | 19.00 | kJ/mol | Joback Method |
| hvap | 55.73 | kJ/mol | Joback Method |
| log10ws | -3.35 | | Crippen Method |
| logp | 3.024 | | Crippen Method |
| mcvol | 155.340 | ml/mol | McGowan Method |
| pc | 4362.63 | kPa | Joback Method |
| rinpol | 1387.00 | | NIST Webbook |
| tb | 607.78 | K | Joback Method |
| tc | 848.93 | K | Joback Method |
| tf | 396.36 | K | Joback Method |
| vc | 0.565 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 302.29 | J/mol×K | 607.78 | Joback Method |
| cpg | 340.54 | J/mol×K | 808.74 | Joback Method |
| cpg | 334.12 | J/mol×K | 768.55 | Joback Method |
| cpg | 327.15 | J/mol×K | 728.36 | Joback Method |
| cpg | 319.57 | J/mol×K | 688.16 | Joback Method |
| cpg | 311.30 | J/mol×K | 647.97 | Joback Method |
| cpg | 346.48 | J/mol×K | 848.93 | Joback Method |
| dvisc | 0.0002206 | Pa×s | 607.78 | Joback Method |
| dvisc | 0.0002807 | Pa×s | 572.54 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0003685 | Pa×s | 537.31 | Joback Method |
| dvisc | 0.0005026 | Pa×s | 502.07 | Joback Method |
| dvisc | 0.0007184 | Pa×s | 466.83 | Joback Method |
| dvisc | 0.0010885 | Pa×s | 431.60 | Joback Method |
| dvisc | 0.0017759 | Pa×s | 396.36 | Joback Method |

# Sources

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|---|---|
| **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=R115821&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |