# Acetic acid, trifluoro-, 3-methylbutyl ester

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|---|---|
| **Other names:** | Trifluoroacetic acid, 3-methylbutyl ester |
| | 3-Methyl-1-butanol, trifluoroacetate |
| | Isopentyl trifluoroacetate |
| **Inchi:** | InChI=1S/C7H11F3O2/c1-5(2)3-4-12-6(11)7(8,9)10/h5H,3-4H2,1-2H3 |
| **InchiKey:** | UOUKEYVAKRKVQA-UHFFFAOYSA-N |
| **Formula:** | C7H11F3O2 |
| **SMILES:** | CC(C)CCOC(=O)C(F)(F)F |
| **Mol. weight [g/mol]:** | 184.16 |
| **CAS:** | 327-69-5 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -809.89 | kJ/mol | Joback Method |
| hf | -1034.97 | kJ/mol | Joback Method |
| hfus | 14.98 | kJ/mol | Joback Method |
| hvap | 36.20 | kJ/mol | Joback Method |
| log10ws | -2.04 | | Crippen Method |
| logp | 2.138 | | Crippen Method |
| mcvol | 122.240 | ml/mol | McGowan Method |
| pc | 2624.46 | kPa | Joback Method |
| rinpol | 759.20 | | NIST Webbook |
| rinpol | 752.10 | | NIST Webbook |
| rinpol | 724.90 | | NIST Webbook |
| tb | 429.99 | K | Joback Method |
| tc | 594.24 | K | Joback Method |
| tf | 230.00 | K | Joback Method |
| vc | 0.488 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 265.92 | J/mol×K | 429.99 | Joback Method |
| cpg | 276.90 | J/mol×K | 457.36 | Joback Method |
| cpg | 287.40 | J/mol×K | 484.74 | Joback Method |

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|---|---|---|---|---|
| cpg | 297.44 | J/mol×K | 512.11 | Joback Method |
| cpg | 307.02 | J/mol×K | 539.49 | Joback Method |
| cpg | 316.16 | J/mol×K | 566.86 | Joback Method |
| cpg | 324.86 | J/mol×K | 594.24 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C327695&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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 |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |