# 1-Trifluoroacetoxy-2-methylpentane

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|---|---|
| **Other names:** | 2-Methyl-1-pentanol, trifluoroacetate |
| | 2-Methylpentyl trifluoroacetate |
| **Inchi:** | InChI=1S/C8H13F3O2/c1-3-4-6(2)5-13-7(12)8(9,10)11/h6H,3-5H2,1-2H3 |
| **InchiKey:** | GBYOBQDQHJMOCS-UHFFFAOYSA-N |
| **Formula:** | C8H13F3O2 |
| **SMILES:** | CCCC(C)COC(=O)C(F)(F)F |
| **Mol. weight [g/mol]:** | 198.18 |
| **CAS:** | 155089-96-6 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -801.47 | kJ/mol | Joback Method |
| hf | -1055.61 | kJ/mol | Joback Method |
| hfus | 17.57 | kJ/mol | Joback Method |
| hvap | 38.42 | kJ/mol | Joback Method |
| log10ws | -2.45 | | Crippen Method |
| logp | 2.528 | | Crippen Method |
| mcvol | 136.330 | ml/mol | McGowan Method |
| pc | 2384.19 | kPa | Joback Method |
| rinpol | 817.40 | | NIST Webbook |
| tb | 452.87 | K | Joback Method |
| tc | 616.33 | K | Joback Method |
| tf | 241.27 | K | Joback Method |
| vc | 0.544 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 307.19 | J/mol×K | 452.87 | Joback Method |
| cpg | 319.14 | J/mol×K | 480.11 | Joback Method |
| cpg | 330.57 | J/mol×K | 507.36 | Joback Method |
| cpg | 341.49 | J/mol×K | 534.60 | Joback Method |
| cpg | 351.92 | J/mol×K | 561.85 | Joback Method |
| cpg | 361.87 | J/mol×K | 589.09 | Joback Method |

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|---|---|---|---|---|
| cpg | 371.35 | J/mol×K | 616.33 | Joback Method |

# 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=C155089966&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |