# Acetic acid, trifluoro-, 2-phenylethyl ester

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|---|---|
| **Other names:** | 1-Trifluoroacetyloxy-2-phenylethane |
| | 2-Phenylethanol, trifluoroacetate |
| **Inchi:** | InChI=1S/C10H9F3O2/c11-10(12,13)9(14)15-7-6-8-4-2-1-3-5-8/h1-5H,6-7H2 |
| **InchiKey:** | JQKSSRRXELCGQS-UHFFFAOYSA-N |
| **Formula:** | C10H9F3O2 |
| **SMILES:** | O=C(OCCc1ccccc1)C(F)(F)F |
| **Mol. weight [g/mol]:** | 218.17 |
| **CAS:** | 55419-66-4 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -669.78 | kJ/mol | Joback Method |
| hf | -855.08 | kJ/mol | Joback Method |
| hfus | 20.31 | kJ/mol | Joback Method |
| hvap | 45.54 | kJ/mol | Joback Method |
| log10ws | -2.64 | | Crippen Method |
| logp | 2.335 | | Crippen Method |
| mcvol | 140.750 | ml/mol | McGowan Method |
| pc | 2721.17 | kPa | Joback Method |
| rinpol | 1086.00 | | NIST Webbook |
| tb | 525.75 | K | Joback Method |
| tc | 720.19 | K | Joback Method |
| tf | 305.23 | K | Joback Method |
| vc | 0.554 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 328.67 | J/mol×K | 525.75 | Joback Method |
| cpg | 341.23 | J/mol×K | 558.16 | Joback Method |
| cpg | 353.00 | J/mol×K | 590.56 | Joback Method |
| cpg | 364.01 | J/mol×K | 622.97 | Joback Method |
| cpg | 374.29 | J/mol×K | 655.38 | Joback Method |
| cpg | 383.87 | J/mol×K | 687.78 | Joback Method |

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|---|---|---|---|---|
| cpg | 392.79 | J/mol×K | 720.19 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C55419664&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 |