# Acetic acid, trifluoro-, 3-methylphenyl ester

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|---|---|
| **Other names:** | 3-Methylphenyl trifluoroacetate |
| | Acetic acid, trifluoro-, m-tolyl ester |
| | Trifluoroacetic acid, 3-methylphenyl ester |
| | Trifluoroacetic acid, 3-tolyl ester |
| **Inchi:** | InChI=1S/C9H7F3O2/c1-6-3-2-4-7(5-6)14-8(13)9(10,11)12/h2-5H,1H3 |
| **InchiKey:** | FXNFSBCSHQEHSB-UHFFFAOYSA-N |
| **Formula:** | C9H7F3O2 |
| **SMILES:** | Cc1cccc(OC(=O)C(F)(F)F)c1 |
| **Mol. weight [g/mol]:** | 204.15 |
| **CAS:** | 1736-09-0 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -687.83 | kJ/mol | Joback Method |
| hf | -845.91 | kJ/mol | Joback Method |
| hfus | 17.33 | kJ/mol | Joback Method |
| hvap | 43.98 | kJ/mol | Joback Method |
| log10ws | -2.92 | | Crippen Method |
| logp | 2.463 | | Crippen Method |
| mcvol | 126.660 | ml/mol | McGowan Method |
| pc | 2966.57 | kPa | Joback Method |
| tb | 507.85 | K | Joback Method |
| tc | 706.00 | K | Joback Method |
| tf | 306.48 | K | Joback Method |
| vc | 0.498 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 284.63 | J/mol×K | 507.85 | Joback Method |
| cpg | 295.99 | J/mol×K | 540.87 | Joback Method |
| cpg | 306.64 | J/mol×K | 573.90 | Joback Method |
| cpg | 316.61 | J/mol×K | 606.92 | Joback Method |
| cpg | 325.92 | J/mol×K | 639.95 | Joback Method |

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|---|---|---|---|---|
| cpg | 334.60 | J/mol×K | 672.97 | Joback Method |
| cpg | 342.69 | J/mol×K | 706.00 | Joback Method |
| hvapt | 47.40 | kJ/mol | 401.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.61363e+01 |
| Coeff. B | -4.64500e+03 |
| Coeff. C | -3.68500e+01 |
| Temperature range (K), min. | 329.93 |
| Temperature range (K), max. | 465.96 |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1736090&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **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 |

# Legend

| | |
|---|---|
| **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 |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |

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|---|---|
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |