# 4-Methylbenzyl 2,2,2-trifluoroacetate

**Inchi:** InChI=1S/C10H9F3O2/c1-7-2-4-8(5-3-7)6-15-9(14)10(11,12)13/h2-5H,6H2,1H3
**InchiKey:** IUUXENSWMSYXPL-UHFFFAOYSA-N
**Formula:** C10H9F3O2
**SMILES:** Cc1ccc(COC(=O)C(F)(F)F)cc1
**Mol. weight [g/mol]:** 218.17

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -679.41 | kJ/mol | Joback Method |
| hf | -866.55 | kJ/mol | Joback Method |
| hfus | 19.92 | kJ/mol | Joback Method |
| hvap | 46.20 | kJ/mol | Joback Method |
| log10ws | -3.19 | | Crippen Method |
| logp | 2.601 | | Crippen Method |
| mcvol | 140.750 | ml/mol | McGowan Method |
| pc | 2679.08 | kPa | Joback Method |
| rinpol | 1102.00 | | NIST Webbook |
| rinpol | 1102.00 | | NIST Webbook |
| tb | 530.73 | K | Joback Method |
| tc | 726.25 | K | Joback Method |
| tf | 317.75 | K | Joback Method |
| vc | 0.554 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 328.54 | J/mol×K | 530.73 | Joback Method |
| cpg | 340.77 | J/mol×K | 563.32 | Joback Method |
| cpg | 352.26 | J/mol×K | 595.90 | Joback Method |
| cpg | 363.03 | J/mol×K | 628.49 | Joback Method |
| cpg | 373.10 | J/mol×K | 661.08 | Joback Method |
| cpg | 382.52 | J/mol×K | 693.66 | Joback Method |
| cpg | 391.31 | J/mol×K | 726.25 | 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=U373211&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 |