# Trifluoroacetic acid, 4-chlorobenzyl ester

**Other names:** 4-Chlorobenzyl alcohol, trifluoroacetate
**Inchi:** InChI=1S/C9H6ClF3O2/c10-7-3-1-6(2-4-7)5-15-8(14)9(11,12)13/h1-4H,5H2
**InchiKey:** WRYXVYBIODRCTM-UHFFFAOYSA-N
**Formula:** C9H6ClF3O2
**SMILES:** O=C(OCc1ccc(Cl)cc1)C(F)(F)F
**Mol. weight [g/mol]:** 238.59
**CAS:** 38696-07-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -699.76 | kJ/mol | Joback Method |
| hf | -861.65 | kJ/mol | Joback Method |
| hfus | 21.53 | kJ/mol | Joback Method |
| hvap | 48.36 | kJ/mol | Joback Method |
| log10ws | -3.40 | | Crippen Method |
| logp | 2.946 | | Crippen Method |
| mcvol | 138.900 | ml/mol | McGowan Method |
| pc | 2850.52 | kPa | Joback Method |
| rinpol | 1184.00 | | NIST Webbook |
| rinpol | 1184.00 | | NIST Webbook |
| tb | 545.28 | K | Joback Method |
| tc | 748.34 | K | Joback Method |
| tf | 336.40 | K | Joback Method |
| vc | 0.547 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 309.43 | J/mol×K | 545.28 | Joback Method |
| cpg | 319.98 | J/mol×K | 579.12 | Joback Method |
| cpg | 329.81 | J/mol×K | 612.97 | Joback Method |
| cpg | 338.95 | J/mol×K | 646.81 | Joback Method |
| cpg | 347.43 | J/mol×K | 680.65 | Joback Method |
| cpg | 355.28 | J/mol×K | 714.49 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 362.52 | J/mol×K | 748.34 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C38696070&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **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 |