# 2,2,2-Trichloroethanol, heptafluorobutyrate

**Inchi:** InChI=1S/C6H2Cl3F7O2/c7-3(8,9)1-18-2(17)4(10,11)5(12,13)6(14,15)16/h1H2
**InchiKey:** BPRJWOQYSBUXBU-UHFFFAOYSA-N
**Formula:** C6H2Cl3F7O2
**SMILES:** O=C(OCC(Cl)(Cl)Cl)C(F)(F)C(F)(F)C(F)(F)F
**Mol. weight [g/mol]:** 345.43

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1622.38 | kJ/mol | Joback Method |
| hf | -1866.96 | kJ/mol | Joback Method |
| hfus | 18.58 | kJ/mol | Joback Method |
| hvap | 40.36 | kJ/mol | Joback Method |
| log10ws | -4.05 | | Crippen Method |
| logp | 3.733 | | Crippen Method |
| mcvol | 151.950 | ml/mol | McGowan Method |
| pc | 2271.90 | kPa | Joback Method |
| rinpol | 902.00 | | NIST Webbook |
| tb | 507.23 | K | Joback Method |
| tc | 683.24 | K | Joback Method |
| tf | 333.11 | K | Joback Method |
| vc | 0.625 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 345.11 | J/mol×K | 507.23 | Joback Method |
| cpg | 353.72 | J/mol×K | 536.57 | Joback Method |
| cpg | 361.52 | J/mol×K | 565.90 | Joback Method |
| cpg | 368.55 | J/mol×K | 595.24 | Joback Method |
| cpg | 374.89 | J/mol×K | 624.57 | Joback Method |
| cpg | 380.56 | J/mol×K | 653.91 | Joback Method |
| cpg | 385.64 | J/mol×K | 683.24 | Joback Method |

# Sources

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|---|---|
| **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=U375579&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |