# 1,1,1-Tris(hydroxymethyl)propane, tri(trifluoroacetate)

**Inchi:** InChI=1S/C12H11F9O6/c1-2-9(3-25-6(22)10(13,14)15,4-26-7(23)11(16,17)18)5-27-8(24)

**InchiKey:** AEKOLUVECIUHSH-UHFFFAOYSA-N

**Formula:** C12H11F9O6

**SMILES:** CCC(COC(=O)C(F)(F)F)(COC(=O)C(F)(F)F)COC(=O)C(F)(F)F

**Mol. weight [g/mol]:** 422.20

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -2393.53 | kJ/mol | Joback Method |
| hf | -2825.40 | kJ/mol | Joback Method |
| hfus | 33.26 | kJ/mol | Joback Method |
| hvap | 57.24 | kJ/mol | Joback Method |
| log10ws | -3.18 | | Crippen Method |
| logp | 2.699 | | Crippen Method |
| mcvol | 218.190 | ml/mol | McGowan Method |
| pc | 1524.69 | kPa | Joback Method |
| rinpol | 1098.00 | | NIST Webbook |
| tb | 683.34 | K | Joback Method |
| tc | 847.33 | K | Joback Method |
| tf | 456.47 | K | Joback Method |
| vc | 0.897 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 645.46 | J/mol×K | 683.34 | Joback Method |
| cpg | 656.04 | J/mol×K | 710.67 | Joback Method |
| cpg | 665.89 | J/mol×K | 738.00 | Joback Method |
| cpg | 675.06 | J/mol×K | 765.33 | Joback Method |
| cpg | 683.57 | J/mol×K | 792.67 | Joback Method |
| cpg | 691.47 | J/mol×K | 820.00 | Joback Method |
| cpg | 698.78 | J/mol×K | 847.33 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U374842&Units=SI |

# 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 |