# 4-Hydroxy-6-oxohept-4-enoic acid, heptafluorobutyrate

**Inchi:** InChI=1S/C11H9F7O5/c1-5(19)4-6(2-3-7(20)21)23-8(22)9(12,13)10(14,15)11(16,17)18/h

**InchiKey:** WOLHNCOTKBYCDQ-XQRVVYSFSA-N

**Formula:** C11H9F7O5

**SMILES:** CC(=O)C=C(CCC(=O)O)OC(=O)C(F)(F)C(F)(F)C(F)(F)F

**Mol. weight [g/mol]:** 354.18

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1870.32 | kJ/mol | Joback Method |
| hf | -2184.15 | kJ/mol | Joback Method |
| hfus | 32.53 | kJ/mol | Joback Method |
| hvap | 69.84 | kJ/mol | Joback Method |
| log10ws | -3.31 | | Crippen Method |
| logp | 2.700 | | Crippen Method |
| mcvol | 190.390 | ml/mol | McGowan Method |
| pc | 2045.61 | kPa | Joback Method |
| rinpol | 1324.00 | | NIST Webbook |
| tb | 716.53 | K | Joback Method |
| tc | 888.85 | K | Joback Method |
| tf | 438.92 | K | Joback Method |
| vc | 0.780 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 552.16 | J/mol×K | 716.53 | Joback Method |
| cpg | 560.54 | J/mol×K | 745.25 | Joback Method |
| cpg | 568.32 | J/mol×K | 773.97 | Joback Method |
| cpg | 575.54 | J/mol×K | 802.69 | Joback Method |
| cpg | 582.26 | J/mol×K | 831.41 | Joback Method |
| cpg | 588.52 | J/mol×K | 860.13 | Joback Method |
| cpg | 594.37 | J/mol×K | 888.85 | 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=U374240&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 |