# 2-Methyl-3-buten-2-ol, heptafluorobutyrate

**Inchi:** InChI=1S/C9H9F7O2/c1-4-6(2,3)18-5(17)7(10,11)8(12,13)9(14,15)16/h4H,1H2,2-3H3
**InchiKey:** OACFSDYVIMZLIH-UHFFFAOYSA-N
**Formula:** C9H9F7O2
**SMILES:** C=CC(C)(C)OC(=O)C(F)(F)C(F)(F)C(F)(F)F
**Mol. weight [g/mol]:** 282.16

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1473.49 | kJ/mol | Joback Method |
| hf | -1756.23 | kJ/mol | Joback Method |
| hfus | 12.48 | kJ/mol | Joback Method |
| hvap | 33.21 | kJ/mol | Joback Method |
| log10ws | -3.71 | | Crippen Method |
| logp | 3.327 | | Crippen Method |
| mcvol | 153.200 | ml/mol | McGowan Method |
| pc | 2005.50 | kPa | Joback Method |
| rinpol | 833.10 | | NIST Webbook |
| rinpol | 833.10 | | NIST Webbook |
| tb | 460.26 | K | Joback Method |
| tc | 619.07 | K | Joback Method |
| tf | 275.40 | K | Joback Method |
| vc | 0.626 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 373.79 | J/mol×K | 460.26 | Joback Method |
| cpg | 386.68 | J/mol×K | 486.73 | Joback Method |
| cpg | 398.72 | J/mol×K | 513.20 | Joback Method |
| cpg | 409.94 | J/mol×K | 539.66 | Joback Method |
| cpg | 420.39 | J/mol×K | 566.13 | Joback Method |
| cpg | 430.10 | J/mol×K | 592.60 | Joback Method |
| cpg | 439.13 | J/mol×K | 619.07 | Joback Method |

# Sources

| | |
|---|---|
| **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=U352696&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |