# valeric acid, 3-methylbut-2-enyl ester

**Inchi:** InChI=1S/C10H18O2/c1-4-5-6-10(11)12-8-7-9(2)3/h7H,4-6,8H2,1-3H3
**InchiKey:** PJMJLIYPHMEZSG-UHFFFAOYSA-N
**Formula:** C10H18O2
**SMILES:** CCCCC(=O)OCC=C(C)C
**Mol. weight [g/mol]:** 170.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.5126 | | Cheméo Relay (1.0) |
| hf | -478.12 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 23.34 | kJ/mol | Joback Method |
| hvap | 56.91 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.71 | eV | Cheméo Relay (1.0) |
| log10ws | -2.96 | | Cheméo Relay (1.0) |
| logp | 2.686 | | Crippen Method |
| mcvol | 154.900 | ml/mol | McGowan Method |
| pc | 2322.54 | kPa | Joback Method |
| rinpol | 1195.60 | | NIST Webbook |
| tb | 470.38 | K | Cheméo Relay (1.0) |
| tc | 645.60 | K | Cheméo Relay (1.0) |
| tf | 210.97 | K | Cheméo Relay (1.0) |
| vc | 0.570 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 350.59 | J/mol×K | 508.53 | Joback Method |
| cpg | 364.62 | J/mol×K | 539.01 | Joback Method |
| cpg | 378.03 | J/mol×K | 569.50 | Joback Method |
| cpg | 390.86 | J/mol×K | 599.98 | Joback Method |
| cpg | 403.11 | J/mol×K | 630.47 | Joback Method |
| cpg | 414.81 | J/mol×K | 660.95 | Joback Method |
| cpg | 425.96 | J/mol×K | 691.44 | Joback Method |

# Sources

| | |
|---|---|
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U292485&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |

# Legend

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|---|---|
| **af:** | Acentric Factor |
| **cpg:** | Ideal gas heat capacity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **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 |