# 3-Methyl-2-butenoic acid, oct-3-en-2-yl ester

**Inchi:** InChI=1S/C13H22O2/c1-5-6-7-8-9-12(4)15-13(14)10-11(2)3/h8-10,12H,5-7H2,1-4H3/b9-
**InchiKey:** UWYBWLYYGHZBJX-CMDGGOBGSA-N
**Formula:** C13H22O2
**SMILES:** CCCCC=CC(C)OC(=O)C=C(C)C
**Mol. weight [g/mol]:** 210.31

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -25.89 | kJ/mol | Joback Method |
| hf | -337.08 | kJ/mol | Joback Method |
| hfus | 27.78 | kJ/mol | Joback Method |
| hvap | 53.30 | kJ/mol | Joback Method |
| log10ws | -3.95 | | Crippen Method |
| logp | 3.631 | | Crippen Method |
| mcvol | 192.870 | ml/mol | McGowan Method |
| pc | 1885.44 | kPa | Joback Method |
| rinpol | 1411.00 | | NIST Webbook |
| rinpol | 1411.00 | | NIST Webbook |
| tb | 580.89 | K | Joback Method |
| tc | 768.98 | K | Joback Method |
| tf | 269.31 | K | Joback Method |
| vc | 0.743 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 476.68 | J/mol×K | 580.89 | Joback Method |
| cpg | 492.79 | J/mol×K | 612.24 | Joback Method |
| cpg | 508.11 | J/mol×K | 643.59 | Joback Method |
| cpg | 522.67 | J/mol×K | 674.94 | Joback Method |
| cpg | 536.50 | J/mol×K | 706.28 | Joback Method |
| cpg | 549.63 | J/mol×K | 737.63 | Joback Method |
| cpg | 562.10 | J/mol×K | 768.98 | 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=U299312&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 |