# But-3-enyl (E)-2-methylbut-2-enoate

**Inchi:** InChI=1S/C9H14O2/c1-4-6-7-11-9(10)8(3)5-2/h4-5H,1,6-7H2,2-3H3/b8-5+
**InchiKey:** DMDOPNKEKJBLCQ-VMPITWQZSA-N
**Formula:** C9H14O2
**SMILES:** C=CCCOC(=O)C(C)=CC
**Mol. weight [g/mol]:** 154.21

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -49.51 | kJ/mol | Joback Method |
| hf | -241.03 | kJ/mol | Joback Method |
| hfus | 19.46 | kJ/mol | Joback Method |
| hvap | 44.15 | kJ/mol | Joback Method |
| log10ws | -2.16 | | Crippen Method |
| logp | 2.072 | | Crippen Method |
| mcvol | 136.510 | ml/mol | McGowan Method |
| pc | 2665.27 | kPa | Joback Method |
| rinpol | 1115.00 | | NIST Webbook |
| tb | 482.33 | K | Joback Method |
| tc | 670.93 | K | Joback Method |
| tf | 242.55 | K | Joback Method |
| vc | 0.525 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 288.43 | J/mol×K | 482.33 | Joback Method |
| cpg | 300.93 | J/mol×K | 513.76 | Joback Method |
| cpg | 312.85 | J/mol×K | 545.20 | Joback Method |
| cpg | 324.21 | J/mol×K | 576.63 | Joback Method |
| cpg | 335.02 | J/mol×K | 608.06 | Joback Method |
| cpg | 345.32 | J/mol×K | 639.49 | Joback Method |
| cpg | 355.10 | J/mol×K | 670.93 | Joback Method |

# Sources

| | |
|---|---|
| **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=U373721&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |