# (Z)-3-Hexenyl 3-methylbutyrate

**Other names:** (Z)-2-Hexenyl isovalerate
**Inchi:** InChI=1S/C11H20O2/c1-4-5-6-7-8-13-11(12)9-10(2)3/h6-7,10H,4-5,8-9H2,1-3H3/b7-6-
**InchiKey:** SAVRWHQEMHIAEB-SREVYHEPSA-N
**Formula:** C11H20O2
**SMILES:** CCCC=CCOC(=O)CC(C)C
**Mol. weight [g/mol]:** 184.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -114.40 | kJ/mol | Joback Method |
| hf | -403.23 | kJ/mol | Joback Method |
| hfus | 23.71 | kJ/mol | Joback Method |
| hvap | 48.81 | kJ/mol | Joback Method |
| log10ws | -2.90 | | Crippen Method |
| logp | 2.932 | | Crippen Method |
| mcvol | 168.990 | ml/mol | McGowan Method |
| pc | 2127.56 | kPa | Joback Method |
| rinpol | 1263.00 | | NIST Webbook |
| rinpol | 1263.00 | | NIST Webbook |
| rinpol | 1245.00 | | NIST Webbook |
| rinpol | 1237.00 | | NIST Webbook |
| rinpol | 1245.00 | | NIST Webbook |
| rinpol | 1237.00 | | NIST Webbook |
| ripol | 1494.00 | | NIST Webbook |
| ripol | 1494.00 | | NIST Webbook |
| ripol | 1477.00 | | NIST Webbook |
| ripol | 1494.00 | | NIST Webbook |
| tb | 531.09 | K | Joback Method |
| tc | 712.68 | K | Joback Method |
| tf | 265.81 | K | Joback Method |
| vc | 0.649 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 397.61 | J/mol×K | 531.09 | Joback Method |
| cpg | 412.58 | J/mol×K | 561.36 | Joback Method |
| cpg | 426.88 | J/mol×K | 591.62 | Joback Method |
| cpg | 440.55 | J/mol×K | 621.89 | Joback Method |
| cpg | 453.60 | J/mol×K | 652.15 | Joback Method |
| cpg | 466.04 | J/mol×K | 682.42 | Joback Method |
| cpg | 477.89 | J/mol×K | 712.68 | Joback Method |
| dvisc | 0.0042170 | Pa×s | 265.81 | Joback Method |
| dvisc | 0.0016682 | Pa×s | 310.02 | Joback Method |
| dvisc | 0.0008318 | Pa×s | 354.24 | Joback Method |
| dvisc | 0.0004840 | Pa×s | 398.45 | Joback Method |
| dvisc | 0.0003138 | Pa×s | 442.66 | Joback Method |
| dvisc | 0.0002201 | Pa×s | 486.88 | Joback Method |
| dvisc | 0.0001638 | Pa×s | 531.09 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R196815&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**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

# Legend

**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**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
**ripol:** Polar retention indices

| | |
|---|---|
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |