# (Z)-3-hexen-2-one

**Inchi:** InChI=1S/C6H10O/c1-3-4-5-6(2)7/h4-5H,3H2,1-2H3/b5-4-
**InchiKey:** LPCWMYHBLXLJJQ-PLNGDYQASA-N
**Formula:** C6H10O
**SMILES:** CCC=CC(C)=O
**Mol. weight [g/mol]:** 98.14

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -49.06 | kJ/mol | Joback Method |
| hf | -162.53 | kJ/mol | Joback Method |
| hfus | 13.10 | kJ/mol | Joback Method |
| hvap | 35.65 | kJ/mol | Joback Method |
| log10ws | -1.47 | | Crippen Method |
| logp | 1.542 | | Crippen Method |
| mcvol | 92.670 | ml/mol | McGowan Method |
| pc | 3547.31 | kPa | Joback Method |
| rinpol | 843.00 | | NIST Webbook |
| rinpol | 843.00 | | NIST Webbook |
| tb | 394.71 | K | Joback Method |
| tc | 581.55 | K | Joback Method |
| tf | 202.23 | K | Joback Method |
| vc | 0.357 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 162.73 | J/mol×K | 394.71 | Joback Method |
| cpg | 172.50 | J/mol×K | 425.85 | Joback Method |
| cpg | 181.81 | J/mol×K | 456.99 | Joback Method |
| cpg | 190.67 | J/mol×K | 488.13 | Joback Method |
| cpg | 199.09 | J/mol×K | 519.27 | Joback Method |
| cpg | 207.09 | J/mol×K | 550.41 | Joback Method |
| cpg | 214.70 | J/mol×K | 581.55 | Joback Method |
| dvisc | 0.0034897 | Pa×s | 202.23 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0016596 | Pa×s | 234.31 | Joback Method |
| dvisc | 0.0009440 | Pa×s | 266.39 | Joback Method |
| dvisc | 0.0006062 | Pa×s | 298.47 | Joback Method |
| dvisc | 0.0004242 | Pa×s | 330.55 | Joback Method |
| dvisc | 0.0003162 | Pa×s | 362.63 | Joback Method |
| dvisc | 0.0002472 | Pa×s | 394.71 | 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=R283088&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

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

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