# Oct-3-enoic acid, but-3-yn-2-yl ester

**Inchi:** InChI=1S/C12H18O2/c1-4-6-7-8-9-10-12(13)14-11(3)5-2/h2,8-9,11H,4,6-7,10H2,1,3H3/b
**InchiKey:** BLTQCWAXHFORDG-CMDGGOBGSA-N
**Formula:** C12H18O2
**SMILES:** C#CC(C)OC(=O)CC=CCCCC
**Mol. weight [g/mol]:** 194.27

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 117.09 | kJ/mol | Joback Method |
| hf | -131.97 | kJ/mol | Joback Method |
| hfus | 29.28 | kJ/mol | Joback Method |
| hvap | 50.89 | kJ/mol | Joback Method |
| log10ws | -3.47 | | Crippen Method |
| logp | 2.688 | | Crippen Method |
| mcvol | 174.480 | ml/mol | McGowan Method |
| pc | 2233.41 | kPa | Joback Method |
| rinpol | 1316.00 | | NIST Webbook |
| rinpol | 1316.00 | | NIST Webbook |
| tb | 544.09 | K | Joback Method |
| tc | 735.18 | K | Joback Method |
| tf | 324.05 | K | Joback Method |
| vc | 0.667 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 407.56 | J/mol×K | 544.09 | Joback Method |
| cpg | 422.14 | J/mol×K | 575.94 | Joback Method |
| cpg | 436.00 | J/mol×K | 607.79 | Joback Method |
| cpg | 449.17 | J/mol×K | 639.64 | Joback Method |
| cpg | 461.68 | J/mol×K | 671.48 | Joback Method |
| cpg | 473.56 | J/mol×K | 703.33 | Joback Method |
| cpg | 484.82 | J/mol×K | 735.18 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U406948&Units=SI |

# 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 |