# Oct-3-enoic acid, 2-methyloct-5-yn-4-yl ester

**Inchi:** InChI=1S/C17H28O2/c1-5-7-9-10-11-13-17(18)19-16(12-8-6-2)14-15(3)4/h10-11,15-16H
**InchiKey:** OZHZRZKKCYELPL-ZHACJKMWSA-N
**Formula:** C17H28O2
**SMILES:** CCC#CC(CC(C)C)OC(=O)CC=CCCCC
**Mol. weight [g/mol]:** 264.40

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 136.48 | kJ/mol | Joback Method |
| hf | -260.05 | kJ/mol | Joback Method |
| hfus | 38.85 | kJ/mol | Joback Method |
| hvap | 63.93 | kJ/mol | Joback Method |
| log10ws | -5.32 | | Crippen Method |
| logp | 4.494 | | Crippen Method |
| mcvol | 244.930 | ml/mol | McGowan Method |
| pc | 1506.98 | kPa | Joback Method |
| rinpol | 1735.00 | | NIST Webbook |
| rinpol | 1735.00 | | NIST Webbook |
| tb | 676.93 | K | Joback Method |
| tc | 869.35 | K | Joback Method |
| tf | 424.53 | K | Joback Method |
| vc | 0.942 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 669.36 | J/mol×K | 676.93 | Joback Method |
| cpg | 687.43 | J/mol×K | 709.00 | Joback Method |
| cpg | 704.58 | J/mol×K | 741.07 | Joback Method |
| cpg | 720.85 | J/mol×K | 773.14 | Joback Method |
| cpg | 736.26 | J/mol×K | 805.21 | Joback Method |
| cpg | 750.85 | J/mol×K | 837.28 | Joback Method |
| cpg | 764.64 | J/mol×K | 869.35 | 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=U406951&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 |