# Undec-10-ynoic acid, 3-methylbut-2-en-1-yl ester

**Inchi:** InChI=1S/C16H26O2/c1-4-5-6-7-8-9-10-11-12-16(17)18-14-13-15(2)3/h1,13H,5-12,14H2

**InchiKey:** PDJHJYUEGLJIHR-UHFFFAOYSA-N

**Formula:** C16H26O2

**SMILES:** C#CCCCCCCCCC(=O)OCC=C(C)C

**Mol. weight [g/mol]:** 250.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 144.66 | kJ/mol | Joback Method |
| hf | -219.04 | kJ/mol | Joback Method |
| hfus | 41.85 | kJ/mol | Joback Method |
| hvap | 60.26 | kJ/mol | Joback Method |
| log10ws | -5.03 | | Crippen Method |
| logp | 4.250 | | Crippen Method |
| mcvol | 230.840 | ml/mol | McGowan Method |
| pc | 1596.17 | kPa | Joback Method |
| rinpol | 1821.00 | | NIST Webbook |
| rinpol | 1821.00 | | NIST Webbook |
| tb | 635.93 | K | Joback Method |
| tc | 818.69 | K | Joback Method |
| tf | 370.17 | K | Joback Method |
| vc | 0.898 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 609.07 | J/mol×K | 635.93 | Joback Method |
| cpg | 625.85 | J/mol×K | 666.39 | Joback Method |
| cpg | 641.83 | J/mol×K | 696.85 | Joback Method |
| cpg | 657.03 | J/mol×K | 727.31 | Joback Method |
| cpg | 671.49 | J/mol×K | 757.77 | Joback Method |
| cpg | 685.25 | J/mol×K | 788.23 | Joback Method |
| cpg | 698.32 | J/mol×K | 818.69 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U406963&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

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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 |