# Undec-10-ynoic acid, 2,7-dimethyloct-1-en-3-yn-5-yl ester

**Inchi:** InChI=1S/C21H32O2/c1-6-7-8-9-10-11-12-13-14-21(22)23-20(17-19(4)5)16-15-18(2)3/h1

**InchiKey:** FLSHKOLQAWMBKK-UHFFFAOYSA-N

**Formula:** C21H32O2

**SMILES:** C#CCCCCCCCCC(=O)OC(C#CC(=C)C)CC(C)C

**Mol. weight [g/mol]:** 316.48

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 392.30 | kJ/mol | Joback Method |
| hf | -52.29 | kJ/mol | Joback Method |
| hfus | 49.39 | kJ/mol | Joback Method |
| hvap | 72.14 | kJ/mol | Joback Method |
| log10ws | -6.79 | | Crippen Method |
| logp | 5.278 | | Crippen Method |
| mcvol | 292.690 | ml/mol | McGowan Method |
| pc | 1260.16 | kPa | Joback Method |
| rinpol | 2090.00 | | NIST Webbook |
| rinpol | 2090.00 | | NIST Webbook |
| tb | 750.97 | K | Joback Method |
| tc | 945.73 | K | Joback Method |
| tf | 505.94 | K | Joback Method |
| vc | 1.129 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 844.69 | J/mol×K | 750.97 | Joback Method |
| cpg | 863.31 | J/mol×K | 783.43 | Joback Method |
| cpg | 880.93 | J/mol×K | 815.89 | Joback Method |
| cpg | 897.59 | J/mol×K | 848.35 | Joback Method |
| cpg | 913.31 | J/mol×K | 880.81 | Joback Method |
| cpg | 928.15 | J/mol×K | 913.27 | Joback Method |
| cpg | 942.14 | J/mol×K | 945.73 | Joback Method |

# Sources

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|---|---|
| **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=U406967&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |