# Hexanoic acid, 3,5,5-trimethyl-, hex-4-yn-3-yl ester

**Inchi:** InChI=1S/C15H26O2/c1-7-9-13(8-2)17-14(16)10-12(3)11-15(4,5)6/h12-13H,8,10-11H2,1

**InchiKey:** PMXBDMXRFMGOQD-UHFFFAOYSA-N

**Formula:** C15H26O2

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

**Mol. weight [g/mol]:** 238.37

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 42.26 | kJ/mol | Joback Method |
| hf | -344.74 | kJ/mol | Joback Method |
| hfus | 26.05 | kJ/mol | Joback Method |
| hvap | 58.22 | kJ/mol | Joback Method |
| log10ws | -4.39 | | Crippen Method |
| logp | 3.794 | | Crippen Method |
| mcvol | 221.050 | ml/mol | McGowan Method |
| pc | 1711.78 | kPa | Joback Method |
| tb | 623.78 | K | Joback Method |
| tc | 823.14 | K | Joback Method |
| tf | 409.49 | K | Joback Method |
| vc | 0.839 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 584.62 | J/mol×K | 623.78 | Joback Method |
| cpg | 603.07 | J/mol×K | 657.01 | Joback Method |
| cpg | 620.55 | J/mol×K | 690.23 | Joback Method |
| cpg | 637.06 | J/mol×K | 723.46 | Joback Method |
| cpg | 652.67 | J/mol×K | 756.69 | Joback Method |
| cpg | 667.38 | J/mol×K | 789.91 | Joback Method |
| cpg | 681.25 | J/mol×K | 823.14 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U406820&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 |

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