# 2-Heptenoic acid, hex-4-yn-3-yl ester

**Inchi:** InChI=1S/C13H20O2/c1-4-7-8-9-11-13(14)15-12(6-3)10-5-2/h9,11-12H,4,6-8H2,1-3H3/b
**InchiKey:** KSIGYFRZAHVJIL-PKNBQFBNSA-N
**Formula:** C13H20O2
**SMILES:** CC#CC(CC)OC(=O)C=CCCCC
**Mol. weight [g/mol]:** 208.30

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 105.24 | kJ/mol | Joback Method |
| hf | -172.21 | kJ/mol | Joback Method |
| hfus | 32.01 | kJ/mol | Joback Method |
| hvap | 55.41 | kJ/mol | Joback Method |
| log10ws | -3.89 | | Crippen Method |
| logp | 3.078 | | Crippen Method |
| mcvol | 188.570 | ml/mol | McGowan Method |
| pc | 2066.12 | kPa | Joback Method |
| rinpol | 1800.00 | | NIST Webbook |
| rinpol | 1800.00 | | NIST Webbook |
| tb | 585.85 | K | Joback Method |
| tc | 783.93 | K | Joback Method |
| tf | 394.45 | K | Joback Method |
| vc | 0.724 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 458.34 | J/mol×K | 585.85 | Joback Method |
| cpg | 474.11 | J/mol×K | 618.86 | Joback Method |
| cpg | 489.12 | J/mol×K | 651.88 | Joback Method |
| cpg | 503.38 | J/mol×K | 684.89 | Joback Method |
| cpg | 516.92 | J/mol×K | 717.91 | Joback Method |
| cpg | 529.75 | J/mol×K | 750.92 | Joback Method |
| cpg | 541.91 | J/mol×K | 783.93 | Joback Method |

# Sources

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|---|---|
| **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=U406941&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |