# Succinic acid, hex-4-yn-3-yl 4-octyl ester

**Inchi:** InChI=1S/C18H30O4/c1-5-9-12-16(11-7-3)22-18(20)14-13-17(19)21-15(8-4)10-6-2/h15-1
**InchiKey:** PBYFPTZKRPPUPO-UHFFFAOYSA-N
**Formula:** C18H30O4
**SMILES:** CC#CC(CC)OC(=O)CCC(=O)OC(CCC)CCCC
**Mol. weight [g/mol]:** 310.43

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -169.24 | kJ/mol | Joback Method |
| hf | -642.71 | kJ/mol | Joback Method |
| hfus | 44.03 | kJ/mol | Joback Method |
| hvap | 75.35 | kJ/mol | Joback Method |
| log10ws | -5.10 | | Crippen Method |
| logp | 4.014 | | Crippen Method |
| mcvol | 270.760 | ml/mol | McGowan Method |
| pc | 1394.37 | kPa | Joback Method |
| rinpol | 1984.00 | | NIST Webbook |
| rinpol | 1984.00 | | NIST Webbook |
| tb | 771.94 | K | Joback Method |
| tc | 964.57 | K | Joback Method |
| tf | 513.04 | K | Joback Method |
| vc | 1.042 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 802.99 | J/mol×K | 771.94 | Joback Method |
| cpg | 820.04 | J/mol×K | 804.05 | Joback Method |
| cpg | 836.09 | J/mol×K | 836.15 | Joback Method |
| cpg | 851.17 | J/mol×K | 868.26 | Joback Method |
| cpg | 865.27 | J/mol×K | 900.36 | Joback Method |
| cpg | 878.41 | J/mol×K | 932.47 | Joback Method |
| cpg | 890.60 | J/mol×K | 964.57 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U389559&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |