

# Succinic acid, hex-4-yn-3-yl 2-methyloct-5-yn-4-yl ester

**Inchi:** InChI=1S/C19H28O4/c1-6-9-11-17(14-15(4)5)23-19(21)13-12-18(20)22-16(8-3)10-7-2/h1-19  
**InchiKey:** FMFDZXLTGIANMC-UHFFFAOYSA-N  
**Formula:** C19H28O4  
**SMILES:** CC#CC(CC)OC(=O)CCC(=O)OC(C#CCC)CC(C)C  
**Mol. weight [g/mol]:** 320.42

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 39.54   | kJ/mol  | Joback Method  |
| hf            | -396.33 | kJ/mol  | Joback Method  |
| hfus          | 46.21   | kJ/mol  | Joback Method  |
| hvap          | 79.34   | kJ/mol  | Joback Method  |
| log10ws       | -5.07   |         | Crippen Method |
| logp          | 3.483   |         | Crippen Method |
| mcvol         | 276.250 | ml/mol  | McGowan Method |
| pc            | 1472.49 | kPa     | Joback Method  |
| rinpol        | 2063.00 |         | NIST Webbook   |
| tb            | 803.38  | K       | Joback Method  |
| tc            | 1011.69 | K       | Joback Method  |
| tf            | 615.41  | K       | Joback Method  |
| vc            | 1.054   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 812.70 | J/mol×K | 803.38          | Joback Method |
| cpg           | 829.64 | J/mol×K | 838.10          | Joback Method |
| cpg           | 845.45 | J/mol×K | 872.82          | Joback Method |
| cpg           | 860.15 | J/mol×K | 907.54          | Joback Method |
| cpg           | 873.75 | J/mol×K | 942.25          | Joback Method |
| cpg           | 886.26 | J/mol×K | 976.97          | Joback Method |
| cpg           | 897.69 | J/mol×K | 1011.69         | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U391028&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391028&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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