

# Succinic acid, but-3-yn-2-yl 2-decyl ester

**Inchi:** InChI=1S/C18H30O4/c1-5-7-8-9-10-11-12-16(4)22-18(20)14-13-17(19)21-15(3)6-2/h2,15  
**InchiKey:** ABCHCHAFEPXTRS-UHFFFAOYSA-N  
**Formula:** C18H30O4  
**SMILES:** C#CC(C)OC(=O)CCC(=O)OC(C)CCCCCCCC  
**Mol. weight [g/mol]:** 310.43

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -148.97 | kJ/mol               | Joback Method  |
| hf            | -623.11 | kJ/mol               | Joback Method  |
| hfus          | 43.88   | kJ/mol               | Joback Method  |
| hvap          | 73.06   | kJ/mol               | Joback Method  |
| log10ws       | -5.10   |                      | Crippen Method |
| logp          | 4.014   |                      | Crippen Method |
| mvol          | 270.760 | ml/mol               | McGowan Method |
| pc            | 1381.96 | kPa                  | Joback Method  |
| rinpol        | 1970.00 |                      | NIST Webbook   |
| rinpol        | 1970.00 |                      | NIST Webbook   |
| tb            | 753.06  | K                    | Joback Method  |
| tc            | 939.36  | K                    | Joback Method  |
| tf            | 453.91  | K                    | Joback Method  |
| vc            | 1.042   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 797.68 | J/mol×K | 753.06          | Joback Method |
| cpg           | 814.46 | J/mol×K | 784.11          | Joback Method |
| cpg           | 830.31 | J/mol×K | 815.16          | Joback Method |
| cpg           | 845.24 | J/mol×K | 846.21          | Joback Method |
| cpg           | 859.29 | J/mol×K | 877.26          | Joback Method |
| cpg           | 872.46 | J/mol×K | 908.31          | Joback Method |
| cpg           | 884.77 | J/mol×K | 939.36          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <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=U390531&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390531&amp;Units=SI</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>rinpola:</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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