

# Succinic acid, tridec-2-yn-1-yl 2-ethoxyethyl ester

**Inchi:** InChI=1S/C21H36O5/c1-3-5-6-7-8-9-10-11-12-13-14-17-25-20(22)15-16-21(23)26-19-18  
**InchiKey:** CAFPM DPIWJWYQM-UHFFFAOYSA-N  
**Formula:** C21H36O5  
**SMILES:** CCCCCCCCCC#CCOC(=O)CCC(=O)OCCOCC  
**Mol. weight [g/mol]:** 368.51

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -244.10 | kJ/mol  | Joback Method  |
| hf            | -826.29 | kJ/mol  | Joback Method  |
| hfus          | 60.03   | kJ/mol  | Joback Method  |
| hvap          | 85.21   | kJ/mol  | Joback Method  |
| log10ws       | -5.22   |         | Crippen Method |
| logp          | 4.424   |         | Crippen Method |
| mcvol         | 318.900 | ml/mol  | McGowan Method |
| pc            | 1111.85 | kPa     | Joback Method  |
| rinpol        | 2595.00 |         | NIST Webbook   |
| tb            | 863.88  | K       | Joback Method  |
| tc            | 1059.75 | K       | Joback Method  |
| tf            | 599.08  | K       | Joback Method  |
| vc            | 1.240   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1010.84 | J/mol×K | 863.88          | Joback Method |
| cpg           | 1028.15 | J/mol×K | 896.52          | Joback Method |
| cpg           | 1044.27 | J/mol×K | 929.17          | Joback Method |
| cpg           | 1059.19 | J/mol×K | 961.81          | Joback Method |
| cpg           | 1072.94 | J/mol×K | 994.46          | Joback Method |
| cpg           | 1085.51 | J/mol×K | 1027.10         | Joback Method |
| cpg           | 1096.91 | J/mol×K | 1059.75         | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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=U390675&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390675&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>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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