

# Succinic acid, hept-2-yl non-3-en-1-yl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C20H36O4/c1-4-6-8-9-10-11-13-17-23-19(21)15-16-20(22)24-18(3)14-12-7-5-2

SBPYYOYUWRTIMT-ZHACJKMWSA-N

C20H36O4

CCCCC=CCCOC(=O)CCC(=O)OC(C)CCCC

340.50

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -272.54 | kJ/mol  | Joback Method  |
| hf            | -833.79 | kJ/mol  | Joback Method  |
| hfus          | 49.81   | kJ/mol  | Joback Method  |
| hvap          | 78.00   | kJ/mol  | Joback Method  |
| log10ws       | -5.88   |         | Crippen Method |
| logp          | 5.348   |         | Crippen Method |
| mcvol         | 303.240 | ml/mol  | McGowan Method |
| pc            | 1121.55 | kPa     | Joback Method  |
| rinpol        | 2238.00 |         | NIST Webbook   |
| rinpol        | 2238.00 |         | NIST Webbook   |
| tb            | 813.30  | K       | Joback Method  |
| tc            | 1000.35 | K       | Joback Method  |
| tf            | 439.40  | K       | Joback Method  |
| vc            | 1.177   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 944.36    | J/mol×K | 813.30          | Joback Method |
| cpg           | 1023.32   | J/mol×K | 969.18          | Joback Method |
| cpg           | 1009.45   | J/mol×K | 938.00          | Joback Method |
| cpg           | 994.65    | J/mol×K | 906.83          | Joback Method |
| cpg           | 978.88    | J/mol×K | 875.65          | Joback Method |
| cpg           | 962.12    | J/mol×K | 844.48          | Joback Method |
| cpg           | 1036.28   | J/mol×K | 1000.35         | Joback Method |
| dvisc         | 0.0000425 | Pa×s    | 813.30          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000574 | Pa×s | 750.98 | Joback Method |
| dvisc | 0.0000819 | Pa×s | 688.67 | Joback Method |
| dvisc | 0.0001253 | Pa×s | 626.35 | Joback Method |
| dvisc | 0.0002106 | Pa×s | 564.03 | Joback Method |
| dvisc | 0.0004027 | Pa×s | 501.72 | Joback Method |
| dvisc | 0.0009257 | Pa×s | 439.40 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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=U391095&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391095&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>                                 |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <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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