

# Succinic acid, 3,7-dimethyloct-6-en-1-yl nonyl ester

|                      |  |
|----------------------|--|
| Inchi:               | InChI=1S/C23H42O4/c1-5-6-7-8-9-10-11-18-26-22(24)15-16-23(25)27-19-17-21(4)14-12 |
| InchiKey:            | YCHMPZZWGODQJG-UHFFFAOYSA-N  |
| Formula:             | C23H42O4   |
| SMILES:              | CCCCCCCCCOC(=O)CCC(=O)OCCC(C)CCC=C(C)C   |
| Mol. weight [g/mol]: | 382.58   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -255.83 | kJ/mol               | Joback Method  |
| hf            | -905.50 | kJ/mol               | Joback Method  |
| hfus          | 56.27   | kJ/mol               | Joback Method  |
| hvap          | 84.75   | kJ/mol               | Joback Method  |
| log10ws       | -6.79   |                      | Crippen Method |
| logp          | 6.376   |                      | Crippen Method |
| mvol          | 345.510 | ml/mol               | McGowan Method |
| pc            | 935.77  | kPa                  | Joback Method  |
| rinpol        | 2568.00 |                      | NIST Webbook   |
| tb            | 881.82  | K                    | Joback Method  |
| tc            | 1079.75 | K                    | Joback Method  |
| tf            | 459.25  | K                    | Joback Method  |
| vc            | 1.347   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1127.93 | J/molxK | 881.82          | Joback Method |
| cpg           | 1146.96 | J/molxK | 914.81          | Joback Method |
| cpg           | 1164.79 | J/molxK | 947.80          | Joback Method |
| cpg           | 1181.46 | J/molxK | 980.79          | Joback Method |
| cpg           | 1197.00 | J/molxK | 1013.77         | Joback Method |
| cpg           | 1211.45 | J/molxK | 1046.76         | Joback Method |
| cpg           | 1224.86 | J/molxK | 1079.75         | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U353343&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353343&amp;Units=SI</a> |
| <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>                     |

# 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>h vap:</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>m cvol:</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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