

# Succinic acid, di(dec-9-en-1-yl) ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C24H42O4/c1-3-5-7-9-11-13-15-17-21-27-23(25)19-20-24(26)28-22-18-16-14- |
| <b>InchiKey:</b>            | PQKFZJXHNIXKBF-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C24H42O4   |
| <b>SMILES:</b>              | C=CCCCCCCCCOC(=O)CCC(=O)OCCCCCCCCC=C   |
| <b>Mol. weight [g/mol]:</b> | 394.59   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -140.96 | kJ/mol               | Joback Method  |
| hf            | -777.43 | kJ/mol               | Joback Method  |
| hfus          | 60.93   | kJ/mol               | Joback Method  |
| hvap          | 85.99   | kJ/mol               | Joback Method  |
| log10ws       | -7.30   |                      | Crippen Method |
| logp          | 6.686   |                      | Crippen Method |
| mvol          | 355.300 | ml/mol               | McGowan Method |
| pc            | 893.20  | kPa                  | Joback Method  |
| rinpol        | 2798.00 |                      | NIST Webbook   |
| rinpol        | 2798.00 |                      | NIST Webbook   |
| tb            | 894.46  | K                    | Joback Method  |
| tc            | 1095.40 | K                    | Joback Method  |
| tf            | 501.04  | K                    | Joback Method  |
| vc            | 1.389   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1159.92   | J/molxK | 894.46          | Joback Method |
| cpg           | 1242.63   | J/molxK | 1061.91         | Joback Method |
| cpg           | 1228.45   | J/molxK | 1028.42         | Joback Method |
| cpg           | 1213.13   | J/molxK | 994.93          | Joback Method |
| cpg           | 1196.63   | J/molxK | 961.44          | Joback Method |
| cpg           | 1178.91   | J/molxK | 927.95          | Joback Method |
| cpg           | 1255.72   | J/molxK | 1095.40         | Joback Method |
| dvisc         | 0.0000340 | Paxs    | 894.46          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000450 | Paxs | 828.89 | Joback Method |
| dvisc | 0.0000626 | Paxs | 763.32 | Joback Method |
| dvisc | 0.0000926 | Paxs | 697.75 | Joback Method |
| dvisc | 0.0001484 | Paxs | 632.18 | Joback Method |
| dvisc | 0.0002655 | Paxs | 566.61 | Joback Method |
| dvisc | 0.0005529 | Paxs | 501.04 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U391253&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391253&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>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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