

# Succinic acid, 2-decyl tridecyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C27H52O4/c1-4-6-8-10-12-13-14-15-16-18-20-24-30-26(28)22-23-27(29)31-25 |
| <b>InchiKey:</b>            | DNTBAYPYTZJNDN-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C27H52O4   |
| <b>SMILES:</b>              | CCCCCCCCCCCCOC(=O)CCC(=O)OC(C)CCCCCCCC   |
| <b>Mol. weight [g/mol]:</b> | 440.70   |

## Physical Properties

| Property code | Value    | Unit                 | Source         |
|---------------|----------|----------------------|----------------|
| gf            | -293.82  | kJ/mol               | Joback Method  |
| hf            | -1095.49 | kJ/mol               | Joback Method  |
| hfus          | 67.74    | kJ/mol               | Joback Method  |
| hvap          | 93.62    | kJ/mol               | Joback Method  |
| log10ws       | -8.96    |                      | Crippen Method |
| logp          | 8.303    |                      | Crippen Method |
| mcvol         | 406.170  | ml/mol               | McGowan Method |
| pc            | 726.53   | kPa                  | Joback Method  |
| rinsol        | 2940.00  |                      | NIST Webbook   |
| tb            | 969.30   | K                    | Joback Method  |
| tc            | 1196.72  | K                    | Joback Method  |
| tf            | 523.37   | K                    | Joback Method  |
| vc            | 1.589    | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1410.04   | J/molxK | 969.30          | Joback Method |
| cpg           | 1501.39   | J/molxK | 1158.81         | Joback Method |
| cpg           | 1486.55   | J/molxK | 1120.91         | Joback Method |
| cpg           | 1470.06   | J/molxK | 1083.01         | Joback Method |
| cpg           | 1451.85   | J/molxK | 1045.11         | Joback Method |
| cpg           | 1431.86   | J/molxK | 1007.20         | Joback Method |
| cpg           | 1514.63   | J/molxK | 1196.72         | Joback Method |
| dvisc         | 0.0000168 | Paxs    | 969.30          | Joback Method |
| dvisc         | 0.0000230 | Paxs    | 894.98          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000331 | Paxs | 820.66 | Joback Method |
| dvisc | 0.0000515 | Paxs | 746.34 | Joback Method |
| dvisc | 0.0000881 | Paxs | 672.01 | Joback Method |
| dvisc | 0.0001723 | Paxs | 597.69 | Joback Method |
| dvisc | 0.0004080 | Paxs | 523.37 | 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=U349433&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U349433&amp;Units=SI</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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