

# Succinic acid, heptadecyl pent-4-enyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C26H48O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-20-24-30-26(28)22-21-2 |
| <b>InchiKey:</b>            | SKBOKGDWEAZGSA-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C26H48O4   |
| <b>SMILES:</b>              | C=CCCCOC(=O)CCC(=O)OCCCCCCCCCCCCCCCCCC   |
| <b>Mol. weight [g/mol]:</b> | 424.66   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -211.96 | kJ/mol               | Joback Method  |
| hf            | -944.14 | kJ/mol               | Joback Method  |
| hfus          | 67.39   | kJ/mol               | Joback Method  |
| hvap          | 91.11   | kJ/mol               | Joback Method  |
| log10ws       | -8.28   |                      | Crippen Method |
| logp          | 7.691   |                      | Crippen Method |
| mcvol         | 387.780 | ml/mol               | McGowan Method |
| pc            | 780.25  | kPa                  | Joback Method  |
| rinsol        | 2919.00 |                      | NIST Webbook   |
| tb            | 943.54  | K                    | Joback Method  |
| tc            | 1160.67 | K                    | Joback Method  |
| tf            | 525.34  | K                    | Joback Method  |
| vc            | 1.520   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1315.55   | J/molxK | 943.54          | Joback Method |
| cpg           | 1404.04   | J/molxK | 1124.48         | Joback Method |
| cpg           | 1389.28   | J/molxK | 1088.30         | Joback Method |
| cpg           | 1373.10   | J/molxK | 1052.11         | Joback Method |
| cpg           | 1355.46   | J/molxK | 1015.92         | Joback Method |
| cpg           | 1336.29   | J/molxK | 979.73          | Joback Method |
| cpg           | 1417.43   | J/molxK | 1160.67         | Joback Method |
| dvisc         | 0.0000233 | Paxs    | 943.54          | Joback Method |
| dvisc         | 0.0000312 | Paxs    | 873.84          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000438 | Paxs | 804.14 | Joback Method |
| dvisc | 0.0000656 | Paxs | 734.44 | Joback Method |
| dvisc | 0.0001071 | Paxs | 664.74 | Joback Method |
| dvisc | 0.0001960 | Paxs | 595.04 | Joback Method |
| dvisc | 0.0004211 | Paxs | 525.34 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U353383&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353383&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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