

# Succinic acid, dec-2-yl cyclopentyl ester

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C19H34O4/c1-3-4-5-6-7-8-11-16(2)22-18(20)14-15-19(21)23-17-12-9-10-13-17 |
| <b>InchiKey:</b>            | SASXKEJJPODCLC-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C19H34O4  |
| <b>SMILES:</b>              | CCCCCCCCC(C)OC(=O)CCC(=O)OC1CCCC1   |
| <b>Mol. weight [g/mol]:</b> | 326.47  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -324.63 | kJ/mol               | Joback Method  |
| hf            | -869.89 | kJ/mol               | Joback Method  |
| hfus          | 40.95   | kJ/mol               | Joback Method  |
| hvap          | 76.07   | kJ/mol               | Joback Method  |
| log10ws       | -5.62   |                      | Crippen Method |
| logp          | 4.935   |                      | Crippen Method |
| mvol          | 282.590 | ml/mol               | McGowan Method |
| pc            | 1310.85 | kPa                  | Joback Method  |
| rinpol        | 2253.00 |                      | NIST Webbook   |
| rinpol        | 2253.00 |                      | NIST Webbook   |
| tb            | 801.54  | K                    | Joback Method  |
| tc            | 995.00  | K                    | Joback Method  |
| tf            | 444.11  | K                    | Joback Method  |
| vc            | 1.083   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 902.10    | J/molxK | 801.54          | Joback Method |
| cpg           | 983.55    | J/molxK | 962.75          | Joback Method |
| cpg           | 969.51    | J/molxK | 930.51          | Joback Method |
| cpg           | 954.37    | J/molxK | 898.27          | Joback Method |
| cpg           | 938.10    | J/molxK | 866.03          | Joback Method |
| cpg           | 920.69    | J/molxK | 833.78          | Joback Method |
| cpg           | 996.51    | J/molxK | 995.00          | Joback Method |
| dvisc         | 0.0000832 | Paxs    | 801.54          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001100 | Paxs | 741.97 | Joback Method |
| dvisc | 0.0001526 | Paxs | 682.40 | Joback Method |
| dvisc | 0.0002254 | Paxs | 622.83 | Joback Method |
| dvisc | 0.0003617 | Paxs | 563.25 | Joback Method |
| dvisc | 0.0006492 | Paxs | 503.68 | Joback Method |
| dvisc | 0.0013628 | Paxs | 444.11 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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=U391380&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391380&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>                                     |

## Legend

|                            |   |
|----------------------------|---|
| <b>cp<sub>g</sub>:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>              | Dynamic viscosity                               |
| <b>g<sub>f</sub>:</b>      | Standard Gibbs free energy of formation         |
| <b>h<sub>f</sub>:</b>      | Enthalpy of formation at standard conditions    |
| <b>h<sub>fus</sub>:</b>    | Enthalpy of fusion at standard conditions       |
| <b>h<sub>vap</sub>:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log<sub>10</sub>ws:</b> | Log <sub>10</sub> of Water solubility in mol/l  |
| <b>log<sub>p</sub>:</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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