

# Succinic acid, cyclohexylmethyl 2-ethylphenyl ester

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C19H26O4/c1-2-16-10-6-7-11-17(16)23-19(21)13-12-18(20)22-14-15-8-4-3-5-9 |
| <b>InchiKey:</b>            | KBIXLOHPEKLDDES-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C19H26O4  |
| <b>SMILES:</b>              | CCc1ccccc1OC(=O)CCC(=O)OCC1CCCCC1   |
| <b>Mol. weight [g/mol]:</b> | 318.41  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -231.51 | kJ/mol               | Joback Method  |
| hf            | -645.71 | kJ/mol               | Joback Method  |
| hfus          | 36.03   | kJ/mol               | Joback Method  |
| hvap          | 79.57   | kJ/mol               | Joback Method  |
| log10ws       | -4.87   |                      | Crippen Method |
| logp          | 4.058   |                      | Crippen Method |
| mcvol         | 258.830 | ml/mol               | McGowan Method |
| pc            | 1694.90 | kPa                  | Joback Method  |
| rinsol        | 2361.00 |                      | NIST Webbook   |
| tb            | 837.91  | K                    | Joback Method  |
| tc            | 1058.86 | K                    | Joback Method  |
| tf            | 494.53  | K                    | Joback Method  |
| vc            | 0.973   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 814.01    | J/molxK | 837.91          | Joback Method |
| cpg           | 831.02    | J/molxK | 874.73          | Joback Method |
| cpg           | 846.57    | J/molxK | 911.56          | Joback Method |
| cpg           | 860.68    | J/molxK | 948.38          | Joback Method |
| cpg           | 873.39    | J/molxK | 985.21          | Joback Method |
| cpg           | 884.72    | J/molxK | 1022.03         | Joback Method |
| cpg           | 894.70    | J/molxK | 1058.86         | Joback Method |
| dvisc         | 0.0007476 | Paxs    | 494.53          | Joback Method |
| dvisc         | 0.0004033 | Paxs    | 551.76          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0002443 | Paxs | 608.99 | Joback Method |
| dvisc | 0.0001613 | Paxs | 666.22 | Joback Method |
| dvisc | 0.0001138 | Paxs | 723.45 | Joback Method |
| dvisc | 0.0000844 | Paxs | 780.68 | Joback Method |
| dvisc | 0.0000653 | Paxs | 837.91 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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=U389950&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U389950&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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