

# Succinic acid, butyl 2-(2-chlorophenoxy)ethyl ester

|                      |  |
|----------------------|--|
| Inchi:               | InChI=1S/C16H21ClO5/c1-2-3-10-21-15(18)8-9-16(19)22-12-11-20-14-7-5-4-6-13(14)17 |
| InchiKey:            | HRAXHLDFUFFIGK-UHFFFAOYSA-N  |
| Formula:             | C16H21ClO5   |
| SMILES:              | CCCCOC(=O)CCC(=O)OCCOc1ccccc1Cl  |
| Mol. weight [g/mol]: | 328.79   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -398.15 | kJ/mol               | Joback Method  |
| hf            | -786.07 | kJ/mol               | Joback Method  |
| hfus          | 41.81   | kJ/mol               | Joback Method  |
| hvap          | 79.26   | kJ/mol               | Joback Method  |
| log10ws       | -3.77   |                      | Crippen Method |
| logp          | 3.385   |                      | Crippen Method |
| mcvol         | 245.530 | ml/mol               | McGowan Method |
| pc            | 1736.11 | kPa                  | Joback Method  |
| rinpol        | 2346.00 |                      | NIST Webbook   |
| rinpol        | 2346.00 |                      | NIST Webbook   |
| tb            | 809.57  | K                    | Joback Method  |
| tc            | 1014.73 | K                    | Joback Method  |
| tf            | 505.49  | K                    | Joback Method  |
| vc            | 0.939   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 702.49    | J/molxK | 809.57          | Joback Method |
| cpg           | 716.09    | J/molxK | 843.76          | Joback Method |
| cpg           | 728.65    | J/molxK | 877.96          | Joback Method |
| cpg           | 740.17    | J/molxK | 912.15          | Joback Method |
| cpg           | 750.66    | J/molxK | 946.34          | Joback Method |
| cpg           | 760.11    | J/molxK | 980.54          | Joback Method |
| cpg           | 768.53    | J/molxK | 1014.73         | Joback Method |
| dvisc         | 0.0005117 | Paxs    | 505.49          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003073 | Paxs | 556.17 | Joback Method |
| dvisc | 0.0002009 | Paxs | 606.85 | Joback Method |
| dvisc | 0.0001403 | Paxs | 657.53 | Joback Method |
| dvisc | 0.0001031 | Paxs | 708.21 | Joback Method |
| dvisc | 0.0000790 | Paxs | 758.89 | Joback Method |
| dvisc | 0.0000625 | Paxs | 809.57 | 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=U381534&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381534&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                                 |

Latest version available from:

<https://www.chemeo.com/cid/120-115-0/Succinic-acid-butyl-2-2-chlorophenoxy-ethyl-ester.pdf>

Generated by Cheméo on 2024-05-02 13:36:04.363122955 +0000 UTC m=+16946213.283700270.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.