

# Succinic acid, 2-methoxybenzyl propyl ester

**Inchi:** InChI=1S/C15H20O5/c1-3-10-19-14(16)8-9-15(17)20-11-12-6-4-5-7-13(12)18-2/h4-7H,3,  
**InchiKey:** OKBKMSRXHYRXHX-UHFFFAOYSA-N  
**Formula:** C15H20O5  
**SMILES:** CCCOC(=O)CCC(=O)OCc1ccccc1OC  
**Mol. weight [g/mol]:** 280.32

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -394.64 | kJ/mol               | Joback Method  |
| hf            | -749.69 | kJ/mol               | Joback Method  |
| hfus          | 35.02   | kJ/mol               | Joback Method  |
| hvap          | 72.64   | kJ/mol               | Joback Method  |
| log10ws       | -3.13   |                      | Crippen Method |
| logp          | 2.472   |                      | Crippen Method |
| mvol          | 219.200 | ml/mol               | McGowan Method |
| pc            | 1945.79 | kPa                  | Joback Method  |
| rinpol        | 2073.00 |                      | NIST Webbook   |
| rinpol        | 2073.00 |                      | NIST Webbook   |
| tb            | 749.26  | K                    | Joback Method  |
| tc            | 951.78  | K                    | Joback Method  |
| tf            | 464.30  | K                    | Joback Method  |
| vc            | 0.834   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 620.91    | J/molxK | 749.26          | Joback Method |
| cpg           | 635.35    | J/molxK | 783.01          | Joback Method |
| cpg           | 648.83    | J/molxK | 816.77          | Joback Method |
| cpg           | 661.35    | J/molxK | 850.52          | Joback Method |
| cpg           | 672.91    | J/molxK | 884.27          | Joback Method |
| cpg           | 683.50    | J/molxK | 918.02          | Joback Method |
| cpg           | 693.12    | J/molxK | 951.78          | Joback Method |
| dvisc         | 0.0006625 | Paxs    | 464.30          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003969 | Paxs | 511.79 | Joback Method |
| dvisc | 0.0002594 | Paxs | 559.29 | Joback Method |
| dvisc | 0.0001812 | Paxs | 606.78 | Joback Method |
| dvisc | 0.0001333 | Paxs | 654.27 | Joback Method |
| dvisc | 0.0001023 | Paxs | 701.77 | Joback Method |
| dvisc | 0.0000811 | Paxs | 749.26 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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=U381204&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381204&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>                                 |

## Legend

|                            |   |
|----------------------------|---|
| <b>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b> | Log <sub>10</sub> of Water solubility in mol/l  |
| <b>logp:</b>               | Octanol/Water partition coefficient             |
| <b>m<sub>cvol</sub>:</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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