

# Succinic acid, 3,5-dinitrobenzyl hexyl ester

**Inchi:** InChI=1S/C17H22N2O8/c1-2-3-4-5-8-26-16(20)6-7-17(21)27-12-13-9-14(18(22)23)11-15  
**InchiKey:** QLHRTTLZGINMGO-UHFFFAOYSA-N  
**Formula:** C17H22N2O8  
**SMILES:** CCCCCCOC(=O)CCC(=O)OCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1  
**Mol. weight [g/mol]:** 382.37

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -211.33 | kJ/mol               | Joback Method  |
| hf            | -691.74 | kJ/mol               | Joback Method  |
| hfus          | 61.34   | kJ/mol               | Joback Method  |
| hvap          | 108.53  | kJ/mol               | Joback Method  |
| log10ws       | -5.56   |                      | Crippen Method |
| logp          | 3.450   |                      | Crippen Method |
| mvol          | 276.350 | ml/mol               | McGowan Method |
| pc            | 1689.34 | kPa                  | Joback Method  |
| rinpol        | 2863.00 |                      | NIST Webbook   |
| rinpol        | 2863.00 |                      | NIST Webbook   |
| tb            | 1081.26 | K                    | Joback Method  |
| tc            | 1328.28 | K                    | Joback Method  |
| tf            | 764.35  | K                    | Joback Method  |
| vc            | 1.091   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 899.22 | J/molxK | 1081.26         | Joback Method |
| cpg           | 907.10 | J/molxK | 1122.43         | Joback Method |
| cpg           | 913.51 | J/molxK | 1163.60         | Joback Method |
| cpg           | 918.50 | J/molxK | 1204.77         | Joback Method |
| cpg           | 922.10 | J/molxK | 1245.94         | Joback Method |
| cpg           | 924.33 | J/molxK | 1287.11         | Joback Method |
| cpg           | 925.24 | J/molxK | 1328.28         | 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=U381098&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381098&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>cpg:</b>     | Ideal gas heat capacity                         |
| <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>hvp:</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>rinp:</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/114-412-7/Succinic-acid-3-5-dinitrobenzyl-hexyl-ester.pdf>

Generated by Cheméo on 2024-04-29 20:01:05.429917068 +0000 UTC m=+16710114.350494384.

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