

# Succinic acid, isobutyl 3-methyl-2-nitrobenzyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C16H21NO6/c1-11(2)9-22-14(18)7-8-15(19)23-10-13-6-4-5-12(3)16(13)17(20) |
| <b>InchiKey:</b>            | BFRSUTTVDINRN-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C16H21NO6  |
| <b>SMILES:</b>              | <chem>Cc1cccc(COC(=O)CCC(=O)OCC(C)C)c1[N+](=O)[O-]</chem>                        |
| <b>Mol. weight [g/mol]:</b> | 323.34   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -257.74 | kJ/mol               | Joback Method  |
| hf            | -665.62 | kJ/mol               | Joback Method  |
| hfus          | 43.87   | kJ/mol               | Joback Method  |
| hvap          | 89.33   | kJ/mol               | Joback Method  |
| log10ws       | -4.31   |                      | Crippen Method |
| logp          | 2.926   |                      | Crippen Method |
| mvol          | 244.840 | ml/mol               | McGowan Method |
| pc            | 1824.72 | kPa                  | Joback Method  |
| rinpol        | 2305.00 |                      | NIST Webbook   |
| rinpol        | 2305.00 |                      | NIST Webbook   |
| tb            | 906.10  | K                    | Joback Method  |
| tc            | 1131.81 | K                    | Joback Method  |
| tf            | 594.47  | K                    | Joback Method  |
| vc            | 0.948   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 754.10 | J/mol×K | 906.10          | Joback Method |
| cpg           | 766.19 | J/mol×K | 943.72          | Joback Method |
| cpg           | 777.05 | J/mol×K | 981.34          | Joback Method |
| cpg           | 786.69 | J/mol×K | 1018.96         | Joback Method |
| cpg           | 795.14 | J/mol×K | 1056.57         | Joback Method |
| cpg           | 802.40 | J/mol×K | 1094.19         | Joback Method |
| cpg           | 808.50 | J/mol×K | 1131.81         | 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=U380965&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380965&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>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>rinpola:</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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