

# Succinic acid, 4-fluoro-3-nitrobenzyl pentyl ester

|                      |  |
|----------------------|--|
| Inchi:               | InChI=1S/C16H20FNO6/c1-2-3-4-9-23-15(19)7-8-16(20)24-11-12-5-6-13(17)14(10-12)18 |
| InchiKey:            | MRGFNDCDFYLBCU-UHFFFAOYSA-N  |
| Formula:             | C16H20FNO6   |
| SMILES:              | CCCCCOC(=O)CCC(=O)OCc1ccc(F)c([N+](=O)[O-])c1                                    |
| Mol. weight [g/mol]: | 341.33   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -450.11 | kJ/mol               | Joback Method  |
| hf            | -856.45 | kJ/mol               | Joback Method  |
| hfus          | 50.47   | kJ/mol               | Joback Method  |
| hvap          | 88.90   | kJ/mol               | Joback Method  |
| log10ws       | -4.83   |                      | Crippen Method |
| logp          | 3.291   |                      | Crippen Method |
| mvol          | 246.610 | ml/mol               | McGowan Method |
| pc            | 1744.82 | kPa                  | Joback Method  |
| rinpol        | 2449.00 |                      | NIST Webbook   |
| rinpol        | 2449.00 |                      | NIST Webbook   |
| tb            | 905.81  | K                    | Joback Method  |
| tc            | 1123.91 | K                    | Joback Method  |
| tf            | 610.06  | K                    | Joback Method  |
| vc            | 0.972   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 760.78 | J/molxK | 905.81          | Joback Method |
| cpg           | 772.39 | J/molxK | 942.16          | Joback Method |
| cpg           | 782.86 | J/molxK | 978.51          | Joback Method |
| cpg           | 792.20 | J/molxK | 1014.86         | Joback Method |
| cpg           | 800.44 | J/molxK | 1051.21         | Joback Method |
| cpg           | 807.59 | J/molxK | 1087.56         | Joback Method |
| cpg           | 813.66 | J/molxK | 1123.91         | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U381019&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381019&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| <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>                     |

# 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                                 |

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