

# Succinic acid, hexyl 3-methylbenzyl ester

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C18H26O4/c1-3-4-5-6-12-21-17(19)10-11-18(20)22-14-16-9-7-8-15(2)13-16/h7 |
| InchiKey:            | UBUNXDJRLNDUEM-UHFFFAOYSA-N                                                       |
| Formula:             | C18H26O4                                                                          |
| SMILES:              | CCCCCOC(=O)CCC(=O)OCc1cccc(C)c1                                                   |
| Mol. weight [g/mol]: | 306.40                                                                            |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -264.38 | kJ/mol  | Joback Method  |
| hf            | -679.39 | kJ/mol  | Joback Method  |
| hfus          | 41.60   | kJ/mol  | Joback Method  |
| hvap          | 76.91   | kJ/mol  | Joback Method  |
| log10ws       | -4.74   |         | Crippen Method |
| logp          | 3.942   |         | Crippen Method |
| mcvol         | 255.600 | ml/mol  | McGowan Method |
| pc            | 1552.45 | kPa     | Joback Method  |
| rinpol        | 2225.00 |         | NIST Webbook   |
| rinpol        | 2225.00 |         | NIST Webbook   |
| tb            | 795.48  | K       | Joback Method  |
| tc            | 995.15  | K       | Joback Method  |
| tf            | 475.88  | K       | Joback Method  |
| vc            | 0.984   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 761.25    | J/mol×K | 795.48          | Joback Method |
| cpg           | 829.35    | J/mol×K | 961.87          | Joback Method |
| cpg           | 817.75    | J/mol×K | 928.59          | Joback Method |
| cpg           | 805.16    | J/mol×K | 895.32          | Joback Method |
| cpg           | 791.55    | J/mol×K | 862.04          | Joback Method |
| cpg           | 776.92    | J/mol×K | 828.76          | Joback Method |
| cpg           | 839.97    | J/mol×K | 995.15          | Joback Method |
| dvisc         | 0.0000720 | Pa×s    | 795.48          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000921 | Pa×s | 742.21 | Joback Method |
| dvisc | 0.0001223 | Pa×s | 688.95 | Joback Method |
| dvisc | 0.0001703 | Pa×s | 635.68 | Joback Method |
| dvisc | 0.0002520 | Pa×s | 582.41 | Joback Method |
| dvisc | 0.0004036 | Pa×s | 529.15 | Joback Method |
| dvisc | 0.0007181 | Pa×s | 475.88 | 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=U382394&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382394&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>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                                 |

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