

# Sebacic acid, butyl tetrahydrofurfuryl ester

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C19H34O5/c1-2-3-14-23-18(20)12-8-6-4-5-7-9-13-19(21)24-16-17-11-10-15-22 |
| InchiKey:            | MGMDAVCFDRXXFT-UHFFFAOYSA-N                                                       |
| Formula:             | C19H34O5                                                                          |
| SMILES:              | CCCCOC(=O)CCCCCCCCC(=O)OCC1CCCO1                                                  |
| Mol. weight [g/mol]: | 342.47                                                                            |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -408.31 | kJ/mol  | Joback Method  |
| hf            | -996.61 | kJ/mol  | Joback Method  |
| hfus          | 52.45   | kJ/mol  | Joback Method  |
| hvap          | 80.97   | kJ/mol  | Joback Method  |
| log10ws       | -4.59   |         | Crippen Method |
| logp          | 4.173   |         | Crippen Method |
| mcvol         | 288.460 | ml/mol  | McGowan Method |
| pc            | 1294.86 | kPa     | Joback Method  |
| rinpol        | 2509.00 |         | NIST Webbook   |
| tb            | 828.93  | K       | Joback Method  |
| tc            | 1022.86 | K       | Joback Method  |
| tf            | 485.68  | K       | Joback Method  |
| vc            | 1.109   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 936.66    | J/mol×K | 828.93          | Joback Method |
| cpg           | 954.37    | J/mol×K | 861.25          | Joback Method |
| cpg           | 970.91    | J/mol×K | 893.57          | Joback Method |
| cpg           | 986.30    | J/mol×K | 925.89          | Joback Method |
| cpg           | 1000.58   | J/mol×K | 958.21          | Joback Method |
| cpg           | 1013.76   | J/mol×K | 990.54          | Joback Method |
| cpg           | 1025.86   | J/mol×K | 1022.86         | Joback Method |
| dvisc         | 0.0009900 | Pa×s    | 485.68          | Joback Method |
| dvisc         | 0.0005193 | Pa×s    | 542.89          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003081 | Pa×s | 600.10 | Joback Method |
| dvisc | 0.0002001 | Pa×s | 657.31 | Joback Method |
| dvisc | 0.0001393 | Pa×s | 714.51 | Joback Method |
| dvisc | 0.0001023 | Pa×s | 771.72 | Joback Method |
| dvisc | 0.0000784 | Pa×s | 828.93 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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>                                 |
| <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=U355720&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355720&amp;Units=SI</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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