# Succinic acid, butyl 2,3-dimethylphenyl ester

**Inchi:** InChI=1S/C16H22O4/c1-4-5-11-19-15(17)9-10-16(18)20-14-8-6-7-12(2)13(14)3/h6-8H,4-

**InchiKey:** XDNSKNTYSNSSFP-UHFFFAOYSA-N

**Formula:** C16H22O4

**SMILES:** CCCCOC(=O)CCC(=O)Oc1cccc(C)c1C

**Mol. weight [g/mol]:** 278.34

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -290.85 | kJ/mol | Joback Method |
| hf | -649.58 | kJ/mol | Joback Method |
| hfus | 36.03 | kJ/mol | Joback Method |
| hvap | 73.12 | kJ/mol | Joback Method |
| log10ws | -4.11 | | Crippen Method |
| logp | 3.332 | | Crippen Method |
| mcvol | 227.420 | ml/mol | McGowan Method |
| pc | 1793.94 | kPa | Joback Method |
| rinpol | 2066.00 | | NIST Webbook |
| tb | 754.70 | K | Joback Method |
| tc | 957.28 | K | Joback Method |
| tf | 465.86 | K | Joback Method |
| vc | 0.872 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 647.65 | J/mol×K | 754.70 | Joback Method |
| cpg | 662.66 | J/mol×K | 788.46 | Joback Method |
| cpg | 676.72 | J/mol×K | 822.23 | Joback Method |
| cpg | 689.83 | J/mol×K | 855.99 | Joback Method |
| cpg | 702.00 | J/mol×K | 889.75 | Joback Method |
| cpg | 713.22 | J/mol×K | 923.52 | Joback Method |
| cpg | 723.52 | J/mol×K | 957.28 | Joback Method |
| dvisc | 0.0007216 | Pa×s | 465.86 | Joback Method |
| dvisc | 0.0004379 | Pa×s | 514.00 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002895 | Pa×s | 562.14 | Joback Method |
| dvisc | 0.0002043 | Pa×s | 610.28 | Joback Method |
| dvisc | 0.0001517 | Pa×s | 658.42 | Joback Method |
| dvisc | 0.0001173 | Pa×s | 706.56 | Joback Method |
| dvisc | 0.0000937 | Pa×s | 754.70 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U349621&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |