# Succinic acid, 3-methylbut-2-yl 2-methoxy-5-methylphenyl ester

**Inchi:** InChI=1S/C17H24O5/c1-11(2)13(4)21-16(18)8-9-17(19)22-15-10-12(3)6-7-14(15)20-5/h6

**InchiKey:** FLBPKSMDNHNDLO-UHFFFAOYSA-N

**Formula:** C17H24O5

**SMILES:** COc1ccc(C)cc1OC(=O)CCC(=O)OC(C)C(C)C

**Mol. weight [g/mol]:** 308.37

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -392.31 | kJ/mol | Joback Method |
| hf | -813.00 | kJ/mol | Joback Method |
| hfus | 32.77 | kJ/mol | Joback Method |
| hvap | 76.98 | kJ/mol | Joback Method |
| log10ws | -4.04 | | Crippen Method |
| logp | 3.277 | | Crippen Method |
| mcvol | 247.380 | ml/mol | McGowan Method |
| pc | 1655.15 | kPa | Joback Method |
| rinpol | 2162.00 | | NIST Webbook |
| rinpol | 2162.00 | | NIST Webbook |
| tb | 799.12 | K | Joback Method |
| tc | 1005.12 | K | Joback Method |
| tf | 469.36 | K | Joback Method |
| vc | 0.933 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 732.96 | J/mol×K | 799.12 | Joback Method |
| cpg | 798.11 | J/mol×K | 970.79 | Joback Method |
| cpg | 787.34 | J/mol×K | 936.45 | Joback Method |
| cpg | 775.44 | J/mol×K | 902.12 | Joback Method |
| cpg | 762.40 | J/mol×K | 867.79 | Joback Method |
| cpg | 748.24 | J/mol×K | 833.45 | Joback Method |
| cpg | 807.75 | J/mol×K | 1005.12 | Joback Method |
| dvisc | 0.0000531 | Pa×s | 799.12 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000686 | Pa×s | 744.16 | Joback Method |
| dvisc | 0.0000924 | Pa×s | 689.20 | Joback Method |
| dvisc | 0.0001310 | Pa×s | 634.24 | Joback Method |
| dvisc | 0.0001985 | Pa×s | 579.28 | Joback Method |
| dvisc | 0.0003280 | Pa×s | 524.32 | Joback Method |
| dvisc | 0.0006097 | Pa×s | 469.36 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U390954&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 |

# Legend

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|---|---|
| **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 |