# Succinic acid, 3-methylbut-2-yl 1-phenylpropyl ester

**Inchi:** InChI=1S/C18H26O4/c1-5-16(15-9-7-6-8-10-15)22-18(20)12-11-17(19)21-14(4)13(2)3/h6
**InchiKey:** BIJZEPKVXUHZMM-UHFFFAOYSA-N
**Formula:** C18H26O4
**SMILES:** CCC(OC(=O)CCC(=O)OC(C)C(C)C)c1ccccc1
**Mol. weight [g/mol]:** 306.40

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -262.07 | kJ/mol | Joback Method |
| hf | -683.76 | kJ/mol | Joback Method |
| hfus | 31.42 | kJ/mol | Joback Method |
| hvap | 75.09 | kJ/mol | Joback Method |
| log10ws | -4.51 | | Crippen Method |
| logp | 4.049 | | Crippen Method |
| mcvol | 255.600 | ml/mol | McGowan Method |
| pc | 1601.28 | kPa | Joback Method |
| rinpol | 2003.00 | | NIST Webbook |
| rinpol | 2003.00 | | NIST Webbook |
| tb | 789.18 | K | Joback Method |
| tc | 995.57 | K | Joback Method |
| tf | 418.36 | K | Joback Method |
| vc | 0.966 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 763.54 | J/mol×K | 789.18 | Joback Method |
| cpg | 833.99 | J/mol×K | 961.18 | Joback Method |
| cpg | 822.13 | J/mol×K | 926.78 | Joback Method |
| cpg | 809.18 | J/mol×K | 892.38 | Joback Method |
| cpg | 795.11 | J/mol×K | 857.98 | Joback Method |
| cpg | 779.91 | J/mol×K | 823.58 | Joback Method |
| cpg | 844.78 | J/mol×K | 995.57 | Joback Method |
| dvisc | 0.0000555 | Pa×s | 789.18 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000758 | Pa×s | 727.38 | Joback Method |
| dvisc | 0.0001096 | Pa×s | 665.57 | Joback Method |
| dvisc | 0.0001709 | Pa×s | 603.77 | Joback Method |
| dvisc | 0.0002949 | Pa×s | 541.97 | Joback Method |
| dvisc | 0.0005856 | Pa×s | 480.16 | Joback Method |
| dvisc | 0.0014242 | Pa×s | 418.36 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U389923&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 |