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

**Inchi:** InChI=1S/C14H24O4/c1-10(2)8-9-17-13(15)6-7-14(16)18-12(5)11(3)4/h8,11-12H,6-7,9H2

**InchiKey:** KXLCDHQOKYYBPH-UHFFFAOYSA-N

**Formula:** C14H24O4

**SMILES:** CC(C)=CCOC(=O)CCC(=O)OC(C)C(C)C

**Mol. weight [g/mol]:** 256.34

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -334.05 | kJ/mol | Joback Method |
| hf | -725.02 | kJ/mol | Joback Method |
| hfus | 29.44 | kJ/mol | Joback Method |
| hvap | 64.33 | kJ/mol | Joback Method |
| log10ws | -3.13 | | Crippen Method |
| logp | 2.864 | | Crippen Method |
| mcvol | 218.700 | ml/mol | McGowan Method |
| pc | 1740.46 | kPa | Joback Method |
| rinpol | 1668.00 | | NIST Webbook |
| rinpol | 1668.00 | | NIST Webbook |
| tb | 675.46 | K | Joback Method |
| tc | 864.48 | K | Joback Method |
| tf | 342.82 | K | Joback Method |
| vc | 0.837 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 600.77 | J/mol×K | 675.46 | Joback Method |
| cpg | 616.61 | J/mol×K | 706.96 | Joback Method |
| cpg | 631.64 | J/mol×K | 738.47 | Joback Method |
| cpg | 645.87 | J/mol×K | 769.97 | Joback Method |
| cpg | 659.31 | J/mol×K | 801.47 | Joback Method |
| cpg | 671.98 | J/mol×K | 832.98 | Joback Method |
| cpg | 683.90 | J/mol×K | 864.48 | Joback Method |

# Sources

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|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U390581&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |

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