

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

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C15H26O4/c1-11(2)9-10-18-13(16)7-8-14(17)19-12(3)15(4,5)6/h9,12H,7-8,10H |
| <b>InchiKey:</b>            | HJWKUTBHCVLGIA-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C15H26O4  |
| <b>SMILES:</b>              | CC(C)=CCOC(=O)CCC(=O)OC(C)C(C)(C)C  |
| <b>Mol. weight [g/mol]:</b> | 270.36  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -320.35 | kJ/mol               | Joback Method  |
| hf            | -749.13 | kJ/mol               | Joback Method  |
| hfus          | 28.14   | kJ/mol               | Joback Method  |
| hvap          | 65.65   | kJ/mol               | Joback Method  |
| log10ws       | -3.55   |                      | Crippen Method |
| logp          | 3.254   |                      | Crippen Method |
| mcvol         | 232.790 | ml/mol               | McGowan Method |
| pc            | 1623.29 | kPa                  | Joback Method  |
| rinsol        | 1722.00 |                      | NIST Webbook   |
| tb            | 695.55  | K                    | Joback Method  |
| tc            | 888.33  | K                    | Joback Method  |
| tf            | 371.51  | K                    | Joback Method  |
| vc            | 0.887   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 657.24 | J/mol×K | 695.55          | Joback Method |
| cpg           | 673.68 | J/mol×K | 727.68          | Joback Method |
| cpg           | 689.20 | J/mol×K | 759.81          | Joback Method |
| cpg           | 703.84 | J/mol×K | 791.94          | Joback Method |
| cpg           | 717.62 | J/mol×K | 824.07          | Joback Method |
| cpg           | 730.59 | J/mol×K | 856.20          | Joback Method |
| cpg           | 742.76 | J/mol×K | 888.33          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <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=U390620&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390620&amp;Units=SI</a> |
| <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>                         |

# Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <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>rinpola:</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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