

# (-)-Dimethyl succinate

|                      |                                                                                                                                      |
|----------------------|--------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | (-)-Dimenthyl succinate<br>Bis((1R,2S,5R)-2-isopropyl-5-methylcyclohexyl) succinate<br>Dimenthyl succinate<br>(-)-Dimethyl succinate |
| Inchi:               | InChI=1S/C24H42O4/c1-15(2)19-9-7-17(5)13-21(19)27-23(25)11-12-24(26)28-22-14-18(                                                     |
| InchiKey:            | YZXZAUAIVAZWFN-UHFFFAOYSA-N                                                                                                          |
| Formula:             | C24H42O4                                                                                                                             |
| SMILES:              | CC1CCC(C(C)C)C(OC(=O)CCC(=O)OC2CC(C)CCC2C(C)C)C1                                                                                     |
| Mol. weight [g/mol]: | 394.60                                                                                                                               |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| hfus          | 44.40   | kJ/mol | Joback Method      |
| hvap          | 108.64  | kJ/mol | Cheméo Relay (1.0) |
| logp          | 5.775   |        | Crippen Method     |
| mcvol         | 342.180 | ml/mol | McGowan Method     |
| tb            | 656.99  | K      | Cheméo Relay (1.0) |
| tc            | 870.27  | K      | Cheméo Relay (1.0) |
| tf            | 307.17  | K      | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1228.01   | J/mol×K | 920.64          | Joback Method |
| cpg           | 1248.56   | J/mol×K | 956.71          | Joback Method |
| cpg           | 1266.98   | J/mol×K | 992.78          | Joback Method |
| cpg           | 1283.28   | J/mol×K | 1028.85         | Joback Method |
| cpg           | 1297.48   | J/mol×K | 1064.92         | Joback Method |
| cpg           | 1309.59   | J/mol×K | 1100.99         | Joback Method |
| cpg           | 1319.62   | J/mol×K | 1137.06         | Joback Method |
| dvisc         | 0.0011986 | Pa×s    | 472.36          | Joback Method |
| dvisc         | 0.0005587 | Pa×s    | 547.07          | Joback Method |
| dvisc         | 0.0003128 | Pa×s    | 621.79          | Joback Method |
| dvisc         | 0.0001984 | Pa×s    | 696.50          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001374 | Pa×s | 771.21 | Joback Method |
| dvisc | 0.0001015 | Pa×s | 845.93 | Joback Method |
| dvisc | 0.0000788 | Pa×s | 920.64 | Joback Method |

## Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C34212594&Units=SI>

Joback Method: [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Cheméo Relay (1.0):

## Legend

|               |                                                 |
|---------------|-------------------------------------------------|
| <b>cpg:</b>   | Ideal gas heat capacity                         |
| <b>dvisc:</b> | Dynamic viscosity                               |
| <b>hfus:</b>  | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>  | Enthalpy of vaporization at standard conditions |
| <b>logp:</b>  | Octanol/Water partition coefficient             |
| <b>mcvol:</b> | McGowan's characteristic volume                 |
| <b>tb:</b>    | Normal Boiling Point Temperature                |
| <b>tc:</b>    | Critical Temperature                            |
| <b>tf:</b>    | Normal melting (fusion) point                   |

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