# di-(1-Methyl-2-methoxybutyl)suberate

**Inchi:** InChI=1S/C18H34O6/c1-13(21-5)15(3)23-17(19)11-9-7-8-10-12-18(20)24-16(4)14(2)22-6
**InchiKey:** YOVKMFKWPJCGRN-UHFFFAOYSA-N
**Formula:** C18H34O6
**SMILES:** COC(C)C(C)OC(=O)CCCCCCC(=O)OC(C)C(C)OC
**Mol. weight [g/mol]:** 346.46

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -586.92 | kJ/mol | Joback Method |
| hf | -1190.01 | kJ/mol | Joback Method |
| hfus | 36.23 | kJ/mol | Joback Method |
| hvap | 77.24 | kJ/mol | Joback Method |
| log10ws | -3.70 | | Crippen Method |
| logp | 3.260 | | Crippen Method |
| mcvol | 291.100 | ml/mol | McGowan Method |
| pc | 1225.98 | kPa | Joback Method |
| rinpol | 1987.00 | | NIST Webbook |
| rinpol | 1987.00 | | NIST Webbook |
| tb | 806.90 | K | Joback Method |
| tc | 994.85 | K | Joback Method |
| tf | 421.40 | K | Joback Method |
| vc | 1.103 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 913.34 | J/mol×K | 806.90 | Joback Method |
| cpg | 930.70 | J/mol×K | 838.23 | Joback Method |
| cpg | 946.93 | J/mol×K | 869.55 | Joback Method |
| cpg | 962.01 | J/mol×K | 900.88 | Joback Method |
| cpg | 975.95 | J/mol×K | 932.20 | Joback Method |
| cpg | 988.74 | J/mol×K | 963.53 | Joback Method |
| cpg | 1000.36 | J/mol×K | 994.85 | Joback Method |
| dvisc | 0.0009946 | Pa×s | 421.40 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0003714 | Pa×s | 485.65 | Joback Method |
| dvisc | 0.0001746 | Pa×s | 549.90 | Joback Method |
| dvisc | 0.0000961 | Pa×s | 614.15 | Joback Method |
| dvisc | 0.0000593 | Pa×s | 678.40 | Joback Method |
| dvisc | 0.0000397 | Pa×s | 742.65 | Joback Method |
| dvisc | 0.0000284 | Pa×s | 806.90 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R541889&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 |