# Dimethyl (Z)-2-n-hexyl-3-methylbutendioate

**Inchi:** InChI=1S/C13H22O4/c1-5-6-7-8-9-11(13(15)17-4)10(2)12(14)16-3/h5-9H2,1-4H3/b11-10
**InchiKey:** SBJHHFISYOOZLE-ZHACJKMWSA-N
**Formula:** C13H22O4
**SMILES:** CCCCCCC(C(=O)OC)=C(C)C(=O)OC
**Mol. weight [g/mol]:** 242.31

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -346.14 | kJ/mol | Joback Method |
| hf | -703.61 | kJ/mol | Joback Method |
| hfus | 32.58 | kJ/mol | Joback Method |
| hvap | 62.96 | kJ/mol | Joback Method |
| log10ws | -2.84 | | Crippen Method |
| logp | 2.619 | | Crippen Method |
| mcvol | 204.610 | ml/mol | McGowan Method |
| pc | 1870.79 | kPa | Joback Method |
| rinpol | 1587.00 | | NIST Webbook |
| rinpol | 1587.00 | | NIST Webbook |
| tb | 653.34 | K | Joback Method |
| tc | 840.46 | K | Joback Method |
| tf | 347.59 | K | Joback Method |
| vc | 0.793 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 546.32 | J/mol×K | 653.34 | Joback Method |
| cpg | 561.30 | J/mol×K | 684.53 | Joback Method |
| cpg | 575.56 | J/mol×K | 715.71 | Joback Method |
| cpg | 589.09 | J/mol×K | 746.90 | Joback Method |
| cpg | 601.92 | J/mol×K | 778.08 | Joback Method |
| cpg | 614.06 | J/mol×K | 809.27 | Joback Method |
| cpg | 625.52 | J/mol×K | 840.46 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R229188&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

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|---|---|
| **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 |