# Dimethylmalonic acid, butyl undecyl ester

**Inchi:** InChI=1S/C20H38O4/c1-5-7-9-10-11-12-13-14-15-17-24-19(22)20(3,4)18(21)23-16-8-6-2
**InchiKey:** IVBGGDXUXRHFAB-UHFFFAOYSA-N
**Formula:** C20H38O4
**SMILES:** CCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCCC
**Mol. weight [g/mol]:** 342.51

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -347.48 | kJ/mol | Joback Method |
| hf | -954.48 | kJ/mol | Joback Method |
| hfus | 45.72 | kJ/mol | Joback Method |
| hvap | 77.13 | kJ/mol | Joback Method |
| log10ws | -5.68 | | Crippen Method |
| logp | 5.430 | | Crippen Method |
| mcvol | 307.540 | ml/mol | McGowan Method |
| pc | 1091.38 | kPa | Joback Method |
| rinpol | 2134.00 | | NIST Webbook |
| tb | 806.35 | K | Joback Method |
| tc | 992.19 | K | Joback Method |
| tf | 461.90 | K | Joback Method |
| vc | 1.192 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 970.19 | J/mol×K | 806.35 | Joback Method |
| cpg | 988.42 | J/mol×K | 837.32 | Joback Method |
| cpg | 1005.60 | J/mol×K | 868.30 | Joback Method |
| cpg | 1021.76 | J/mol×K | 899.27 | Joback Method |
| cpg | 1036.94 | J/mol×K | 930.24 | Joback Method |
| cpg | 1051.16 | J/mol×K | 961.22 | Joback Method |
| cpg | 1064.44 | J/mol×K | 992.19 | Joback Method |
| dvisc | 0.0008014 | Pa×s | 461.90 | Joback Method |
| dvisc | 0.0003752 | Pa×s | 519.31 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002043 | Pa×s | 576.72 | Joback Method |
| dvisc | 0.0001242 | Pa×s | 634.12 | Joback Method |
| dvisc | 0.0000820 | Pa×s | 691.53 | Joback Method |
| dvisc | 0.0000577 | Pa×s | 748.94 | Joback Method |
| dvisc | 0.0000427 | Pa×s | 806.35 | 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=U361778&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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