# Dimethylmalonic acid, isobutyl octadecyl ester

**Inchi:** InChI=1S/C27H52O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-30-25(28)27(
**InchiKey:** AQPXBCSSKAULPN-UHFFFAOYSA-N
**Formula:** C27H52O4
**SMILES:** CCCCCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCC(C)C
**Mol. weight [g/mol]:** 440.70

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -290.98 | kJ/mol | Joback Method |
| hf | -1104.24 | kJ/mol | Joback Method |
| hfus | 60.32 | kJ/mol | Joback Method |
| hvap | 92.32 | kJ/mol | Joback Method |
| log10ws | -8.37 | | Crippen Method |
| logp | 8.017 | | Crippen Method |
| mcvol | 406.170 | ml/mol | McGowan Method |
| pc | 734.03 | kPa | Joback Method |
| rinpol | 2786.00 | | NIST Webbook |
| tb | 966.07 | K | Joback Method |
| tc | 1188.14 | K | Joback Method |
| tf | 525.79 | K | Joback Method |
| vc | 1.579 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1409.68 | J/mol×K | 966.07 | Joback Method |
| cpg | 1431.04 | J/mol×K | 1003.08 | Joback Method |
| cpg | 1450.77 | J/mol×K | 1040.09 | Joback Method |
| cpg | 1468.94 | J/mol×K | 1077.10 | Joback Method |
| cpg | 1485.63 | J/mol×K | 1114.11 | Joback Method |
| cpg | 1500.92 | J/mol×K | 1151.12 | Joback Method |
| cpg | 1514.88 | J/mol×K | 1188.14 | Joback Method |
| dvisc | 0.0003661 | Pa×s | 525.79 | Joback Method |
| dvisc | 0.0001487 | Pa×s | 599.17 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000735 | Pa×s | 672.55 | Joback Method |
| dvisc | 0.0000418 | Pa×s | 745.93 | Joback Method |
| dvisc | 0.0000262 | Pa×s | 819.31 | Joback Method |
| dvisc | 0.0000178 | Pa×s | 892.69 | Joback Method |
| dvisc | 0.0000128 | Pa×s | 966.07 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U361666&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 |
| **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 |