# Decanedioic acid, dimethyl ester

| | |
|---|---|
| **Other names:** | Decanedioic acid, methyl ester |
| | Dimethyl decanedioate |
| | Dimethyl octane-1,8-dicarboxylate |
| | Dimethyl sebacate |
| | Methyl sebacate |
| | Sebacic acid, dimethyl ester |
| | decadioic acid, dimethyl ester |
| | decandioic acid, dimethyl ester |
| **Inchi:** | InChI=1S/C12H22O4/c1-15-11(13)9-7-5-3-4-6-8-10-12(14)16-2/h3-10H2,1-2H3 |
| **InchiKey:** | ALOUNLDAKADEEB-UHFFFAOYSA-N |
| **Formula:** | C12H22O4 |
| **SMILES:** | COC(=O)CCCCCCCCC(=O)OC |
| **Mol. weight [g/mol]:** | 230.30 |
| **CAS:** | 106-79-6 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -6844.20 | kJ/mol | NIST Webbook |
| gf | -417.68 | kJ/mol | Joback Method |
| hf | -780.61 | kJ/mol | Joback Method |
| hfus | 32.41 | kJ/mol | Joback Method |
| hvap | 86.40 ± 0.30 | kJ/mol | NIST Webbook |
| log10ws | -3.28 | | Aqueous Solubility Prediction Method |
| logp | 2.453 | | Crippen Method |
| mcvol | 194.820 | ml/mol | McGowan Method |
| pc | 2080.00 | kPa | Vapor Pressures, Enthalpies of Vaporization, and Critical Parameters of a Series of Linear Aliphatic Dimethyl Esters of Dicarboxylic Acids |
| rinpol | 1612.00 | | NIST Webbook |
| rinpol | 279.26 | | NIST Webbook |
| rinpol | 1650.00 | | NIST Webbook |
| rinpol | 283.00 | | NIST Webbook |
| rinpol | 282.90 | | NIST Webbook |
| rinpol | 1634.00 | | NIST Webbook |
| rinpol | 1645.00 | | NIST Webbook |

| | | | |
|---|---|---|---|
| rinpol | 1615.00 | | NIST Webbook |
| rinpol | 1613.00 | | NIST Webbook |
| rinpol | 1616.00 | | NIST Webbook |
| rinpol | 1616.00 | | NIST Webbook |
| rinpol | 1613.00 | | NIST Webbook |
| rinpol | 1613.00 | | NIST Webbook |
| rinpol | 1613.00 | | NIST Webbook |
| rinpol | 1614.00 | | NIST Webbook |
| rinpol | 1646.00 | | NIST Webbook |
| rinpol | 1627.00 | | NIST Webbook |
| rinpol | 282.90 | | NIST Webbook |
| rinpol | 1611.00 | | NIST Webbook |
| rinpol | 1612.00 | | NIST Webbook |
| rinpol | 1611.00 | | NIST Webbook |
| rinpol | 1619.00 | | NIST Webbook |
| rinpol | 1631.00 | | NIST Webbook |
| rinpol | 1620.00 | | NIST Webbook |
| rinpol | 1649.00 | | NIST Webbook |
| rinpol | 1619.00 | | NIST Webbook |
| rinpol | 1650.50 | | NIST Webbook |
| rinpol | 1650.00 | | NIST Webbook |
| rinpol | 1616.00 | | NIST Webbook |
| rinpol | 1612.00 | | NIST Webbook |
| rinpol | 1645.00 | | NIST Webbook |
| rinpol | 283.00 | | NIST Webbook |
| ripol | 2212.00 | | NIST Webbook |
| ripol | 2220.00 | | NIST Webbook |
| ripol | 2195.00 | | NIST Webbook |
| tb | 626.54 | K | Joback Method |
| tc | 803.91 | K | Joback Method |
| tf | 301.20 ± 2.00 | K | NIST Webbook |
| tf | 299.95 ± 0.50 | K | NIST Webbook |
| tf | 300.20 ± 1.50 | K | NIST Webbook |
| tf | 299.60 ± 2.00 | K | NIST Webbook |
| tf | 299.55 ± 0.50 | K | NIST Webbook |
| tf | 303.53 | K | Aqueous Solubility Prediction Method |
| vc | 0.755 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| cpg | 515.96 | J/mol×K | 626.54 | Joback Method |
| cpg | 530.51 | J/mol×K | 656.10 | Joback Method |
| cpg | 544.42 | J/mol×K | 685.66 | Joback Method |
| cpg | 557.71 | J/mol×K | 715.23 | Joback Method |
| cpg | 570.37 | J/mol×K | 744.79 | Joback Method |
| cpg | 582.39 | J/mol×K | 774.35 | Joback Method |
| cpg | 593.78 | J/mol×K | 803.91 | Joback Method |
| dvisc | 0.0017118 | Pa×s | 369.32 | Joback Method |
| dvisc | 0.0009273 | Pa×s | 412.19 | Joback Method |
| dvisc | 0.0005638 | Pa×s | 455.06 | Joback Method |
| dvisc | 0.0003735 | Pa×s | 497.93 | Joback Method |
| dvisc | 0.0002641 | Pa×s | 540.80 | Joback Method |
| dvisc | 0.0001965 | Pa×s | 583.67 | Joback Method |
| dvisc | 0.0001522 | Pa×s | 626.54 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 431.20 | K | 1.30 | NIST Webbook |
| tbrp | 448.20 | K | 2.70 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 2.07093e+01 |
| Coeff. B | -1.19940e+04 |
| Coeff. C | 1.79937e+02 |
| Temperature range (K), min. | 407.38 |
| Temperature range (K), max. | 599.00 |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C106796&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Vapor Pressures, Enthalpies of Vaporization, and Critical Parameters of a Series of Linear Aliphatic Dimethyl Esters of Dicarboxylic Acids:** | https://www.doi.org/10.1021/je0602418 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

| | |
|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **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 |
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |