

# Octanedioic acid, 3-methyl-, dimethyl ester

<b>Inchi:</b>	InChI=1S/C11H20O4/c1-9(8-11(13)15-3)6-4-5-7-10(12)14-2/h9H,4-8H2,1-3H3
<b>InchiKey:</b>	XXILFTORDPJBLE-UHFFFAOYSA-N
<b>Formula:</b>	C11H20O4
<b>SMILES:</b>	COC(=O)CCCC(C)CC(=O)OC
<b>Mol. weight [g/mol]:</b>	216.27
<b>CAS:</b>	54576-15-7

## Physical Properties

Property code	Value	Unit	Source
gf	-428.54	kJ/mol	Joback Method
hf	-765.25	kJ/mol	Joback Method
hfus	26.30	kJ/mol	Joback Method
hvap	58.00	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.919		Crippen Method
mvol	180.730	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	1453.00		NIST Webbook
rinpol	1453.00		NIST Webbook
tb	603.22	K	Joback Method
tc	784.89	K	Joback Method
tf	343.05	K	Joback Method
vc	0.694	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.43	J/mol×K	603.22	Joback Method
cpg	479.63	J/mol×K	633.50	Joback Method
cpg	493.21	J/mol×K	663.78	Joback Method
cpg	506.18	J/mol×K	694.06	Joback Method
cpg	518.53	J/mol×K	724.34	Joback Method
cpg	530.27	J/mol×K	754.61	Joback Method
cpg	541.38	J/mol×K	784.89	Joback Method

dvisc	0.0022861	Paxs	343.05	Joback Method
dvisc	0.0011425	Paxs	386.41	Joback Method
dvisc	0.0006567	Paxs	429.77	Joback Method
dvisc	0.0004178	Paxs	473.13	Joback Method
dvisc	0.0002868	Paxs	516.50	Joback Method
dvisc	0.0002087	Paxs	559.86	Joback Method
dvisc	0.0001589	Paxs	603.22	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C54576157&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C54576157&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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