

# Dimethylmalonic acid, octadecyl undecyl ester

**Inchi:** InChI=1S/C34H66O4/c1-5-7-9-11-13-15-16-17-18-19-20-21-23-25-27-29-31-38-33(36)34  
**InchiKey:** HGYPUJYOCLTDEK-UHFFFAOYSA-N  
**Formula:** C34H66O4  
**SMILES:** CCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCCCCCCCCCC  
**Mol. weight [g/mol]:** 538.89

## Physical Properties

Property code	Value	Unit	Source
gf	-229.60	kJ/mol	Joback Method
hf	-1243.44	kJ/mol	Joback Method
hfus	81.98	kJ/mol	Joback Method
hvap	108.29	kJ/mol	Joback Method
log10ws	-11.54		Crippen Method
logp	10.891		Crippen Method
mcvol	504.800	ml/mol	McGowan Method
pc	523.41	kPa	Joback Method
rinsol	3511.00		NIST Webbook
tb	1126.67	K	Joback Method
tc	1450.76	K	Joback Method
tf	619.68	K	Joback Method
vc	1.976	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1869.38	J/molxK	1126.67	Joback Method
cpg	1897.20	J/molxK	1180.69	Joback Method
cpg	1921.85	J/molxK	1234.70	Joback Method
cpg	1943.66	J/molxK	1288.72	Joback Method
cpg	1962.94	J/molxK	1342.73	Joback Method
cpg	1980.01	J/molxK	1396.75	Joback Method
cpg	1995.20	J/molxK	1450.76	Joback Method
dvisc	0.0001136	Paxs	619.68	Joback Method
dvisc	0.0000476	Paxs	704.18	Joback Method

dvisc	0.0000241	Paxs	788.68	Joback Method
dvisc	0.0000139	Paxs	873.17	Joback Method
dvisc	0.0000088	Paxs	957.67	Joback Method
dvisc	0.0000060	Paxs	1042.17	Joback Method
dvisc	0.0000044	Paxs	1126.67	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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=U361787&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361787&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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