

# Dimethylmalonic acid, isohexyl 4-octyl ester

<b>Inchi:</b>	InChI=1S/C19H36O4/c1-7-9-13-16(11-8-2)23-18(21)19(5,6)17(20)22-14-10-12-15(3)4/h1
<b>InchiKey:</b>	XTAJKZCWQUWQFK-UHFFFAOYSA-N
<b>Formula:</b>	C19H36O4
<b>SMILES:</b>	CCCCC(CCC)OC(=O)C(C)(C)C(=O)OCCCC(C)C
<b>Mol. weight [g/mol]:</b>	328.49

## Physical Properties

Property code	Value	Unit	Source
gf	-360.78	kJ/mol	Joback Method
hf	-944.40	kJ/mol	Joback Method
hfus	36.08	kJ/mol	Joback Method
hvap	74.13	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.894		Crippen Method
mcvol	293.450	ml/mol	McGowan Method
pc	1176.85	kPa	Joback Method
rinsol	1860.00		NIST Webbook
tb	782.59	K	Joback Method
tc	969.42	K	Joback Method
tf	420.63	K	Joback Method
vc	1.125	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.15	J/molxK	782.59	Joback Method
cpg	929.33	J/molxK	813.73	Joback Method
cpg	946.47	J/molxK	844.87	Joback Method
cpg	962.57	J/molxK	876.00	Joback Method
cpg	977.69	J/molxK	907.14	Joback Method
cpg	991.84	J/molxK	938.28	Joback Method
cpg	1005.05	J/molxK	969.42	Joback Method
dvisc	0.0013462	Paxs	420.63	Joback Method
dvisc	0.0005259	Paxs	480.96	Joback Method

dvisc	0.0002533	Paxs	541.28	Joback Method
dvisc	0.0001413	Paxs	601.61	Joback Method
dvisc	0.0000876	Paxs	661.94	Joback Method
dvisc	0.0000589	Paxs	722.26	Joback Method
dvisc	0.0000421	Paxs	782.59	Joback Method

## Sources

<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=U361733&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361733&amp;Units=SI</a>
<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>

## 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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