

# Dimethylmalonic acid, cis-4-methylcyclohexyl trans-4-methylcyclohexyl ester

<b>Inchi:</b>	InChI=1S/C19H32O4/c1-13-5-9-15(10-6-13)22-17(20)19(3,4)18(21)23-16-11-7-14(2)8-12
<b>InchiKey:</b>	ZVDVSV AEMPCQCL-UHFFFAOYSA-N
<b>Formula:</b>	C19H32O4
<b>SMILES:</b>	CC1CCC(OC(=O)C(C)(C)C(=O)OC2CCC(C)CC2)CC1
<b>Mol. weight [g/mol]:</b>	324.45

## Physical Properties

Property code	Value	Unit	Source
gf	-322.42	kJ/mol	Joback Method
hf	-865.88	kJ/mol	Joback Method
hfus	28.94	kJ/mol	Joback Method
hvap	75.14	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.256		Crippen Method
mvol	271.730	ml/mol	McGowan Method
pc	1494.19	kPa	Joback Method
rinpol	2149.00		NIST Webbook
rinpol	2149.00		NIST Webbook
tb	813.23	K	Joback Method
tc	1037.22	K	Joback Method
tf	456.91	K	Joback Method
vc	1.000	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.85	J/molxK	813.23	Joback Method
cpg	931.39	J/molxK	850.56	Joback Method
cpg	951.09	J/molxK	887.89	Joback Method
cpg	968.98	J/molxK	925.23	Joback Method
cpg	985.10	J/molxK	962.56	Joback Method
cpg	999.49	J/molxK	999.89	Joback Method
cpg	1012.19	J/molxK	1037.22	Joback Method
dvisc	0.0012971	Paxs	456.91	Joback Method

dvisc	0.0006362	Paxs	516.30	Joback Method
dvisc	0.0003614	Paxs	575.68	Joback Method
dvisc	0.0002283	Paxs	635.07	Joback Method
dvisc	0.0001559	Paxs	694.46	Joback Method
dvisc	0.0001131	Paxs	753.84	Joback Method
dvisc	0.0000860	Paxs	813.23	Joback Method

## Sources

<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=U363893&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U363893&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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