

# Dimethylmalonic acid, cis-4-methylcyclohexyl isohexyl ester

<b>Inchi:</b>	InChI=1S/C18H32O4/c1-13(2)7-6-12-21-16(19)18(4,5)17(20)22-15-10-8-14(3)9-11-15/h1
<b>InchiKey:</b>	GKABQZJQDGTTPN-UHFFFAOYSA-N
<b>Formula:</b>	C18H32O4
<b>SMILES:</b>	CC(C)CCCOC(=O)C(C)(C)C(=O)OC1CCC(C)CC1
<b>Mol. weight [g/mol]:</b>	312.44

## Physical Properties

Property code	Value	Unit	Source
gf	-350.02	kJ/mol	Joback Method
hf	-884.50	kJ/mol	Joback Method
hfus	29.92	kJ/mol	Joback Method
hvap	72.41	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.114		Crippen Method
mcvol	268.500	ml/mol	McGowan Method
pc	1418.64	kPa	Joback Method
rinsol	2008.00		NIST Webbook
rinsol	2008.00		NIST Webbook
tb	775.03	K	Joback Method
tc	978.85	K	Joback Method
tf	427.50	K	Joback Method
vc	1.006	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.63	J/molxK	775.03	Joback Method
cpg	935.87	J/molxK	944.88	Joback Method
cpg	921.41	J/molxK	910.91	Joback Method
cpg	905.68	J/molxK	876.94	Joback Method
cpg	888.66	J/molxK	842.97	Joback Method
cpg	870.32	J/molxK	809.00	Joback Method
cpg	949.11	J/molxK	978.85	Joback Method
dvisc	0.0000691	Paxs	775.03	Joback Method

dvisc	0.0000935	Paxs	717.11	Joback Method
dvisc	0.0001333	Paxs	659.19	Joback Method
dvisc	0.0002035	Paxs	601.26	Joback Method
dvisc	0.0003402	Paxs	543.34	Joback Method
dvisc	0.0006426	Paxs	485.42	Joback Method
dvisc	0.0014425	Paxs	427.50	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=U363878&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U363878&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>
<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>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>h<sub>vap</sub>:</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>log<sub>p</sub>:</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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