

# Dimethylmalonic acid, isohexyl 3-methylphenyl ester

<b>Inchi:</b>	InChI=1S/C18H26O4/c1-13(2)8-7-11-21-16(19)18(4,5)17(20)22-15-10-6-9-14(3)12-15/h6
<b>InchiKey:</b>	FJWPCOBOQFDTCA-UHFFFAOYSA-N
<b>Formula:</b>	C18H26O4
<b>SMILES:</b>	<chem>Cc1cccc(OC(=O)C(C)(C)C(=O)OCCCC(C)C)c1</chem>
<b>Mol. weight [g/mol]:</b>	306.40

## Physical Properties

Property code	Value	Unit	Source
gf	-263.98	kJ/mol	Joback Method
hf	-693.42	kJ/mol	Joback Method
hfus	30.66	kJ/mol	Joback Method
hvap	75.23	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.906		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	1983.00		NIST Webbook
tb	791.81	K	Joback Method
tc	1001.25	K	Joback Method
tf	463.30	K	Joback Method
vc	0.967	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.36	J/molxK	791.81	Joback Method
cpg	779.50	J/molxK	826.72	Joback Method
cpg	794.50	J/molxK	861.62	Joback Method
cpg	808.40	J/molxK	896.53	Joback Method
cpg	821.22	J/molxK	931.44	Joback Method
cpg	833.02	J/molxK	966.34	Joback Method
cpg	843.81	J/molxK	1001.25	Joback Method
dvisc	0.0007844	Paxs	463.30	Joback Method
dvisc	0.0003954	Paxs	518.05	Joback Method

dvisc	0.0002272	Paxs	572.80	Joback Method
dvisc	0.0001438	Paxs	627.55	Joback Method
dvisc	0.0000980	Paxs	682.31	Joback Method
dvisc	0.0000707	Paxs	737.06	Joback Method
dvisc	0.0000533	Paxs	791.81	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=U363613&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U363613&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>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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