

# Dimethylmalonic acid, heptyl octyl ester

<b>Inchi:</b>	InChI=1S/C20H38O4/c1-5-7-9-11-13-15-17-24-19(22)20(3,4)18(21)23-16-14-12-10-8-6-2
<b>InchiKey:</b>	CMTUYYPWBPYIIR-UHFFFAOYSA-N
<b>Formula:</b>	C20H38O4
<b>SMILES:</b>	CCCCCCCCOC(=O)C(C)(C)C(=O)OCCCCCCC
<b>Mol. weight [g/mol]:</b>	342.51

## Physical Properties

Property code	Value	Unit	Source
gf	-347.48	kJ/mol	Joback Method
hf	-954.48	kJ/mol	Joback Method
hfus	45.72	kJ/mol	Joback Method
hvap	77.13	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	5.430		Crippen Method
mvol	307.540	ml/mol	McGowan Method
pc	1091.38	kPa	Joback Method
rinpol	2116.00		NIST Webbook
rinpol	2116.00		NIST Webbook
tb	806.35	K	Joback Method
tc	992.19	K	Joback Method
tf	461.90	K	Joback Method
vc	1.192	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.19	J/molxK	806.35	Joback Method
cpg	1051.16	J/molxK	961.22	Joback Method
cpg	1036.94	J/molxK	930.24	Joback Method
cpg	1021.76	J/molxK	899.27	Joback Method
cpg	1005.60	J/molxK	868.30	Joback Method
cpg	988.42	J/molxK	837.32	Joback Method
cpg	1064.44	J/molxK	992.19	Joback Method
dvisc	0.0000427	Paxs	806.35	Joback Method

dvisc	0.0000577	Paxs	748.94	Joback Method
dvisc	0.0000820	Paxs	691.53	Joback Method
dvisc	0.0001242	Paxs	634.12	Joback Method
dvisc	0.0002043	Paxs	576.72	Joback Method
dvisc	0.0003752	Paxs	519.31	Joback Method
dvisc	0.0008014	Paxs	461.90	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U361674&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361674&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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