

# Dimethylmalonic acid, di(2-pentyl) ester

<b>Inchi:</b>	InChI=1S/C15H28O4/c1-7-9-11(3)18-13(16)15(5,6)14(17)19-12(4)10-8-2/h11-12H,7-10H
<b>InchiKey:</b>	ABNHNUGFNGXQTK-UHFFFAOYSA-N
<b>Formula:</b>	C15H28O4
<b>SMILES:</b>	CCCC(C)OC(=O)C(C)(C)C(=O)OC(C)CCC
<b>Mol. weight [g/mol]:</b>	272.38

## Physical Properties

Property code	Value	Unit	Source
gf	-394.46	kJ/mol	Joback Method
hf	-861.84	kJ/mol	Joback Method
hfus	25.72	kJ/mol	Joback Method
hvap	65.22	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.476		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
rinpol	1571.00		NIST Webbook
tb	691.07	K	Joback Method
tc	878.32	K	Joback Method
tf	375.55	K	Joback Method
vc	0.900	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.58	J/mol×K	691.07	Joback Method
cpg	756.61	J/mol×K	847.11	Joback Method
cpg	743.16	J/mol×K	815.90	Joback Method
cpg	728.85	J/mol×K	784.70	Joback Method
cpg	713.66	J/mol×K	753.49	Joback Method
cpg	697.58	J/mol×K	722.28	Joback Method
cpg	769.22	J/mol×K	878.32	Joback Method
dvisc	0.0000764	Paxs	691.07	Joback Method
dvisc	0.0001064	Paxs	638.48	Joback Method

dvisc	0.0001571	Paxs	585.90	Joback Method
dvisc	0.0002507	Paxs	533.31	Joback Method
dvisc	0.0004430	Paxs	480.72	Joback Method
dvisc	0.0009002	Paxs	428.14	Joback Method
dvisc	0.0022315	Paxs	375.55	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=U361592&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361592&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>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

Latest version available from:

<https://www.chemeo.com/cid/22-358-0/Dimethylmalonic-acid-di-2-pentyl-ester.pdf>

Generated by Cheméo on 2024-04-23 21:52:56.243042723 +0000 UTC m=+16198425.163620038.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.