

# Dimethylmalonic acid, 4-acetylphenyl nonyl ester

Inchi:	InChI=1S/C22H32O5/c1-5-6-7-8-9-10-11-16-26-20(24)22(3,4)21(25)27-19-14-12-18(13-1
InchiKey:	UUTVVKRMRUUPTB-UHFFFAOYSA-N
Formula:	C22H32O5
SMILES:	CCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]:	376.49

## Physical Properties

Property code	Value	Unit	Source
gf	-356.78	kJ/mol	Joback Method
hf	-883.28	kJ/mol	Joback Method
hfus	46.15	kJ/mol	Joback Method
hvap	91.27	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	5.115		Crippen Method
mvol	313.530	ml/mol	McGowan Method
pc	1239.83	kPa	Joback Method
rinpol	2616.00		NIST Webbook
rinpol	2616.00		NIST Webbook
tb	937.64	K	Joback Method
tc	1152.88	K	Joback Method
tf	573.31	K	Joback Method
vc	1.202	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.44	J/molxK	937.64	Joback Method
cpg	1075.22	J/molxK	1117.01	Joback Method
cpg	1065.16	J/molxK	1081.13	Joback Method
cpg	1054.01	J/molxK	1045.26	Joback Method
cpg	1041.70	J/molxK	1009.39	Joback Method
cpg	1028.20	J/molxK	973.51	Joback Method
cpg	1084.23	J/molxK	1152.88	Joback Method
dvisc	0.0000301	Paxs	937.64	Joback Method

dvisc	0.0000392	Paxs	876.92	Joback Method
dvisc	0.0000531	Paxs	816.20	Joback Method
dvisc	0.0000756	Paxs	755.47	Joback Method
dvisc	0.0001145	Paxs	694.75	Joback Method
dvisc	0.0001878	Paxs	634.03	Joback Method
dvisc	0.0003420	Paxs	573.31	Joback Method

## Sources

<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=U363703&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U363703&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>

## 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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