

# Malonic acid, 3-hexyl propyl ester

<b>Inchi:</b>	InChI=1S/C12H22O4/c1-4-7-10(6-3)16-12(14)9-11(13)15-8-5-2/h10H,4-9H2,1-3H3
<b>InchiKey:</b>	LDTBLYPPJNBKMS-UHFFFAOYSA-N
<b>Formula:</b>	C12H22O4
<b>SMILES:</b>	CCCOC(=O)CC(=O)OC(CC)CCC
<b>Mol. weight [g/mol]:</b>	230.30

## Physical Properties

Property code	Value	Unit	Source
gf	-420.12	kJ/mol	Joback Method
hf	-785.89	kJ/mol	Joback Method
hfus	28.89	kJ/mol	Joback Method
hvap	60.23	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.452		Crippen Method
mcvol	194.820	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	1469.00		NIST Webbook
tb	626.10	K	Joback Method
tc	806.33	K	Joback Method
tf	354.32	K	Joback Method
vc	0.750	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.38	J/molxK	626.10	Joback Method
cpg	583.91	J/molxK	776.29	Joback Method
cpg	571.72	J/molxK	746.25	Joback Method
cpg	558.88	J/molxK	716.21	Joback Method
cpg	545.37	J/molxK	686.18	Joback Method
cpg	531.21	J/molxK	656.14	Joback Method
cpg	595.44	J/molxK	806.33	Joback Method
dvisc	0.0001418	Paxs	626.10	Joback Method
dvisc	0.0001868	Paxs	580.80	Joback Method

dvisc	0.0002579	Paxs	535.51	Joback Method
dvisc	0.0003780	Paxs	490.21	Joback Method
dvisc	0.0005987	Paxs	444.91	Joback Method
dvisc	0.0010527	Paxs	399.62	Joback Method
dvisc	0.0021379	Paxs	354.32	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=U349118&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U349118&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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