

# Malonic acid, 2-methylpent-3-yl propyl ester

<b>Inchi:</b>	InChI=1S/C12H22O4/c1-5-7-15-11(13)8-12(14)16-10(6-2)9(3)4/h9-10H,5-8H2,1-4H3
<b>InchiKey:</b>	VJLVHFOAYMMTTH-UHFFFAOYSA-N
<b>Formula:</b>	C12H22O4
<b>SMILES:</b>	CCCOC(=O)CC(=O)OC(CC)C(C)C
<b>Mol. weight [g/mol]:</b>	230.30

## Physical Properties

Property code	Value	Unit	Source
gf	-422.56	kJ/mol	Joback Method
hf	-791.17	kJ/mol	Joback Method
hfus	25.36	kJ/mol	Joback Method
hvap	59.84	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.308		Crippen Method
mcvol	194.820	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
rinqol	1434.00		NIST Webbook
tb	625.66	K	Joback Method
tc	808.87	K	Joback Method
tf	339.32	K	Joback Method
vc	0.744	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.81	J/molxK	625.66	Joback Method
cpg	585.47	J/molxK	778.33	Joback Method
cpg	573.11	J/molxK	747.80	Joback Method
cpg	560.07	J/molxK	717.26	Joback Method
cpg	546.34	J/molxK	686.73	Joback Method
cpg	531.92	J/molxK	656.19	Joback Method
cpg	597.13	J/molxK	808.87	Joback Method
dvisc	0.0001321	Paxs	625.66	Joback Method
dvisc	0.0001778	Paxs	577.94	Joback Method

dvisc	0.0002525	Paxs	530.21	Joback Method
dvisc	0.0003843	Paxs	482.49	Joback Method
dvisc	0.0006416	Paxs	434.77	Joback Method
dvisc	0.0012154	Paxs	387.04	Joback Method
dvisc	0.0027555	Paxs	339.32	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U349045&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U349045&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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