

# Malonic acid, 3,3-dimethylbut-2-yl hexyl ester

**Inchi:** InChI=1S/C15H28O4/c1-6-7-8-9-10-18-13(16)11-14(17)19-12(2)15(3,4)5/h12H,6-11H2,1  
**InchiKey:** OOAAKQWEBIYRJT-UHFFFAOYSA-N  
**Formula:** C15H28O4  
**SMILES:** CCCCCCOC(=O)CC(=O)OC(C)C(C)(C)C  
**Mol. weight [g/mol]:** 272.38

## Physical Properties

Property code	Value	Unit	Source
gf	-392.02	kJ/mol	Joback Method
hf	-856.56	kJ/mol	Joback Method
hfus	29.24	kJ/mol	Joback Method
hvap	65.61	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.478		Crippen Method
mvol	237.090	ml/mol	McGowan Method
pc	1551.22	kPa	Joback Method
rinpol	1688.00		NIST Webbook
rinpol	1688.00		NIST Webbook
tb	691.51	K	Joback Method
tc	876.12	K	Joback Method
tf	390.55	K	Joback Method
vc	0.906	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.11	J/molxK	691.51	Joback Method
cpg	696.84	J/molxK	722.28	Joback Method
cpg	712.70	J/molxK	753.05	Joback Method
cpg	727.68	J/molxK	783.82	Joback Method
cpg	741.83	J/molxK	814.59	Joback Method
cpg	755.14	J/molxK	845.35	Joback Method
cpg	767.65	J/molxK	876.12	Joback Method
dvisc	0.0017437	Paxs	390.55	Joback Method

dvisc	0.0007852	Paxs	440.71	Joback Method
dvisc	0.0004162	Paxs	490.87	Joback Method
dvisc	0.0002481	Paxs	541.03	Joback Method
dvisc	0.0001615	Paxs	591.19	Joback Method
dvisc	0.0001124	Paxs	641.35	Joback Method
dvisc	0.0000825	Paxs	691.51	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=U347207&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U347207&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>cp<sub>g</sub>:</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>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rin<sub>pol</sub>:</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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