

# Malonic acid, isohexyl 4-methylpent-2-yl ester

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

## Physical Properties

Property code	Value	Unit	Source
gf	-399.74	kJ/mol	Joback Method
hf	-858.37	kJ/mol	Joback Method
hfus	29.61	kJ/mol	Joback Method
hvap	66.13	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.334		Crippen Method
mvol	237.090	ml/mol	McGowan Method
pc	1547.57	kPa	Joback Method
rinpol	1647.00		NIST Webbook
rinpol	1647.00		NIST Webbook
tb	693.86	K	Joback Method
tc	876.51	K	Joback Method
tf	358.13	K	Joback Method
vc	0.905	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.70	J/molxK	693.86	Joback Method
cpg	754.34	J/molxK	846.06	Joback Method
cpg	740.89	J/molxK	815.62	Joback Method
cpg	726.61	J/molxK	785.18	Joback Method
cpg	711.49	J/molxK	754.74	Joback Method
cpg	695.52	J/molxK	724.30	Joback Method
cpg	766.97	J/molxK	876.51	Joback Method
dvisc	0.0000837	Paxs	693.86	Joback Method

dvisc	0.0001159	Paxs	637.90	Joback Method
dvisc	0.0001709	Paxs	581.95	Joback Method
dvisc	0.0002735	Paxs	526.00	Joback Method
dvisc	0.0004895	Paxs	470.04	Joback Method
dvisc	0.0010257	Paxs	414.08	Joback Method
dvisc	0.0027078	Paxs	358.13	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U349334&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U349334&amp;Units=SI</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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