

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

Inchi:	InChI=1S/C13H24O4/c1-9(2)8-16-11(14)7-12(15)17-10(3)13(4,5)6/h9-10H,7-8H2,1-6H3
InchiKey:	HVSCYIDCHWGOHX-UHFFFAOYSA-N
Formula:	C13H24O4
SMILES:	CC(C)COC(=O)CC(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]:	244.33

## Physical Properties

Property code	Value	Unit	Source
gf	-411.30	kJ/mol	Joback Method
hf	-820.56	kJ/mol	Joback Method
hfus	20.54	kJ/mol	Joback Method
hvap	60.77	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.554		Crippen Method
mvol	208.910	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinpol	1454.00		NIST Webbook
rinpol	1454.00		NIST Webbook
tb	645.31	K	Joback Method
tc	835.59	K	Joback Method
tf	353.01	K	Joback Method
vc	0.788	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.06	J/molxK	645.31	Joback Method
cpg	588.28	J/molxK	677.02	Joback Method
cpg	603.65	J/molxK	708.74	Joback Method
cpg	618.18	J/molxK	740.45	Joback Method
cpg	631.88	J/molxK	772.16	Joback Method
cpg	644.77	J/molxK	803.87	Joback Method
cpg	656.88	J/molxK	835.59	Joback Method
dvisc	0.0028022	Paxs	353.01	Joback Method

dvisc	0.0011521	Paxs	401.73	Joback Method
dvisc	0.0005741	Paxs	450.44	Joback Method
dvisc	0.0003278	Paxs	499.16	Joback Method
dvisc	0.0002067	Paxs	547.88	Joback Method
dvisc	0.0001406	Paxs	596.59	Joback Method
dvisc	0.0001013	Paxs	645.31	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=U347202&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U347202&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>

## 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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