

# Malonic acid diisopropyl ester

<b>Other names:</b>	Propanedioic acid, bis(1-methylethyl) ester diisopropyl malonate dipropan-2-yl propanedioate propanedioic acid, 1,3-bis(1-methylethyl) ester
<b>Inchi:</b>	InChI=1S/C9H16O4/c1-6(2)12-8(10)5-9(11)13-7(3)4/h6-7H,5H2,1-4H3
<b>InchiKey:</b>	QRVSDVDFJFKYKA-UHFFFAOYSA-N
<b>Formula:</b>	C9H16O4
<b>SMILES:</b>	CC(C)OC(=O)CC(=O)OC(C)C
<b>Mol. weight [g/mol]:</b>	188.22
<b>CAS:</b>	13195-64-7

## Physical Properties

Property code	Value	Unit	Source
gf	-447.82	kJ/mol	Joback Method
hf	-729.25	kJ/mol	Joback Method
hfus	61.40	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	64.81	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	64.49	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	64.20	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	63.90	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	63.60	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids

hfus	63.30	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	63.00	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	62.70	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	62.40	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	62.20	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	62.09	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	61.90	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	61.21	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	61.60	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	61.50	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	61.81	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hvap	53.16	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.280		Crippen Method
mcvol	152.550	ml/mol	McGowan Method

pc	2566.29	kPa	Joback Method
rinpol	1116.00		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1113.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1108.00		NIST Webbook
tb	557.02	K	Joback Method
tc	745.99	K	Joback Method
tf	305.51	K	Joback Method
vc	0.576	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.76	J/mol×K	557.02	Joback Method
cpg	428.24	J/mol×K	714.49	Joback Method
cpg	417.44	J/mol×K	683.00	Joback Method
cpg	406.09	J/mol×K	651.50	Joback Method
cpg	394.19	J/mol×K	620.01	Joback Method
cpg	381.74	J/mol×K	588.51	Joback Method
cpg	438.48	J/mol×K	745.99	Joback Method
dvisc	0.0001840	Paxs	557.02	Joback Method
dvisc	0.0002454	Paxs	515.10	Joback Method
dvisc	0.0003443	Paxs	473.18	Joback Method
dvisc	0.0005161	Paxs	431.26	Joback Method
dvisc	0.0008440	Paxs	389.35	Joback Method
dvisc	0.0015540	Paxs	347.43	Joback Method
dvisc	0.0033834	Paxs	305.51	Joback Method

## Sources

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids:**

<https://www.doi.org/10.1016/j.fluid.2011.07.007>

**McGowan Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C13195647&Units=SI>

# 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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