

# Malonic acid, decyl 2-decyl ester

<b>Inchi:</b>	InChI=1S/C23H44O4/c1-4-6-8-10-12-13-15-17-19-26-22(24)20-23(25)27-21(3)18-16-14-
<b>InchiKey:</b>	VKUBOIFDCHKUXMH-UHFFFAOYSA-N
<b>Formula:</b>	C23H44O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)CC(=O)OC(C)CCCCCCCC
<b>Mol. weight [g/mol]:</b>	384.59

## Physical Properties

Property code	Value	Unit	Source
gf	-327.50	kJ/mol	Joback Method
hf	-1012.93	kJ/mol	Joback Method
hfus	57.38	kJ/mol	Joback Method
hvap	84.72	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	6.743		Crippen Method
mcvol	349.810	ml/mol	McGowan Method
pc	903.97	kPa	Joback Method
rinpol	2510.00		NIST Webbook
rinpol	2510.00		NIST Webbook
tb	877.78	K	Joback Method
tc	1074.72	K	Joback Method
tf	478.29	K	Joback Method
vc	1.365	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1154.96	J/molxK	877.78	Joback Method
cpg	1240.32	J/molxK	1041.89	Joback Method
cpg	1225.74	J/molxK	1009.07	Joback Method
cpg	1209.94	J/molxK	976.25	Joback Method
cpg	1192.90	J/molxK	943.43	Joback Method
cpg	1174.58	J/molxK	910.60	Joback Method
cpg	1253.72	J/molxK	1074.72	Joback Method
dvisc	0.0000313	Paxs	877.78	Joback Method

dvisc	0.0000424	Paxs	811.20	Joback Method
dvisc	0.0000607	Paxs	744.62	Joback Method
dvisc	0.0000932	Paxs	678.03	Joback Method
dvisc	0.0001571	Paxs	611.45	Joback Method
dvisc	0.0003008	Paxs	544.87	Joback Method
dvisc	0.0006901	Paxs	478.29	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=U349095&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U349095&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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