

# Malonic acid, 2-chloropropyl tridecyl ester

<b>Inchi:</b>	InChI=1S/C19H35ClO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-23-18(21)15-19(22)24-16-17(2)
<b>InchiKey:</b>	XQULABOIZJGPFB-UHFFFAOYSA-N
<b>Formula:</b>	C19H35ClO4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)CC(=O)OCC(C)Cl
<b>Mol. weight [g/mol]:</b>	362.93

## Physical Properties

Property code	Value	Unit	Source
gf	-373.11	kJ/mol	Joback Method
hf	-946.11	kJ/mol	Joback Method
hfus	51.21	kJ/mol	Joback Method
hvap	80.20	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	5.401		Crippen Method
mvol	305.690	ml/mol	McGowan Method
pc	1126.83	kPa	Joback Method
rinpol	2407.00		NIST Webbook
rinpol	2407.00		NIST Webbook
tb	823.69	K	Joback Method
tc	1011.93	K	Joback Method
tf	463.13	K	Joback Method
vc	1.190	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.05	J/molxK	823.69	Joback Method
cpg	958.06	J/molxK	855.06	Joback Method
cpg	974.02	J/molxK	886.44	Joback Method
cpg	988.97	J/molxK	917.81	Joback Method
cpg	1002.91	J/molxK	949.19	Joback Method
cpg	1015.87	J/molxK	980.56	Joback Method
cpg	1027.85	J/molxK	1011.93	Joback Method
dvisc	0.0008626	Paxs	463.13	Joback Method

dvisc	0.0004054	Paxs	523.22	Joback Method
dvisc	0.0002226	Paxs	583.32	Joback Method
dvisc	0.0001367	Paxs	643.41	Joback Method
dvisc	0.0000912	Paxs	703.50	Joback Method
dvisc	0.0000649	Paxs	763.60	Joback Method
dvisc	0.0000485	Paxs	823.69	Joback Method

## Sources

<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=U349035&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U349035&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>hvap:</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>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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