

# Dimethylmalonic acid, 4-chlorophenyl undecyl ester

<b>Inchi:</b>	InChI=1S/C22H33ClO4/c1-4-5-6-7-8-9-10-11-12-17-26-20(24)22(2,3)21(25)27-19-15-13
<b>InchiKey:</b>	KLTOJAXRXCYBJN-UHFFFAOYSA-N
<b>Formula:</b>	C22H33ClO4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	396.95

## Physical Properties

Property code	Value	Unit	Source
gf	-239.79	kJ/mol	Joback Method
hf	-786.44	kJ/mol	Joback Method
hfus	48.74	kJ/mol	Joback Method
hvap	88.90	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	6.346		Crippen Method
mvol	324.200	ml/mol	McGowan Method
pc	1156.93	kPa	Joback Method
rinpol	2584.00		NIST Webbook
tb	921.20	K	Joback Method
tc	1133.31	K	Joback Method
tf	553.30	K	Joback Method
vc	1.246	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.74	J/molxK	921.20	Joback Method
cpg	1040.19	J/molxK	956.55	Joback Method
cpg	1054.44	J/molxK	991.90	Joback Method
cpg	1067.54	J/molxK	1027.26	Joback Method
cpg	1079.53	J/molxK	1062.61	Joback Method
cpg	1090.48	J/molxK	1097.96	Joback Method
cpg	1100.43	J/molxK	1133.31	Joback Method
dvisc	0.0003423	Paxs	553.30	Joback Method
dvisc	0.0001817	Paxs	614.62	Joback Method

dvisc	0.0001082	Paxs	675.93	Joback Method
dvisc	0.0000702	Paxs	737.25	Joback Method
dvisc	0.0000487	Paxs	798.57	Joback Method
dvisc	0.0000356	Paxs	859.88	Joback Method
dvisc	0.0000271	Paxs	921.20	Joback Method

## Sources

<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=U361981&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361981&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>
<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>

## 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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