

# Dimethylmalonic acid, 2,4-dichloro-6-formylphenyl undecyl ester

Inchi:	InChI=1S/C23H32Cl2O5/c1-4-5-6-7-8-9-10-11-12-13-29-21(27)23(2,3)22(28)30-20-17(16)
InchiKey:	MJEHTVKSYSYCOKMC-UHFFFAOYSA-N
Formula:	C23H32Cl2O5
SMILES:	CCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1c(Cl)cc(Cl)cc1C=O
Mol. weight [g/mol]:	459.40

## Physical Properties

Property code	Value	Unit	Source
gf	-362.08	kJ/mol	Joback Method
hf	-931.34	kJ/mol	Joback Method
hfus	57.04	kJ/mol	Joback Method
hvap	103.56	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	6.811		Crippen Method
mvol	352.100	ml/mol	McGowan Method
pc	1089.94	kPa	Joback Method
rinpol	2922.00		NIST Webbook
rinpol	2922.00		NIST Webbook
tb	1040.13	K	Joback Method
tc	1273.42	K	Joback Method
tf	661.53	K	Joback Method
vc	1.367	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1116.42	J/molxK	1040.13	Joback Method
cpg	1128.86	J/molxK	1079.01	Joback Method
cpg	1139.98	J/molxK	1117.89	Joback Method
cpg	1149.81	J/molxK	1156.77	Joback Method
cpg	1158.43	J/molxK	1195.66	Joback Method
cpg	1165.90	J/molxK	1234.54	Joback Method
cpg	1172.27	J/molxK	1273.42	Joback Method
dvisc	0.0001780	Paxs	661.53	Joback Method

dvisc	0.0001070	Paxs	724.63	Joback Method
dvisc	0.0000698	Paxs	787.73	Joback Method
dvisc	0.0000485	Paxs	850.83	Joback Method
dvisc	0.0000354	Paxs	913.93	Joback Method
dvisc	0.0000269	Paxs	977.03	Joback Method
dvisc	0.0000212	Paxs	1040.13	Joback Method

## Sources

<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>
<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=U363640&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U363640&amp;Units=SI</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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