

# Dimethylmalonic acid, decyl 2,5-dichlorophenyl ester

Inchi:	InChI=1S/C21H30Cl2O4/c1-4-5-6-7-8-9-10-11-14-26-19(24)21(2,3)20(25)27-18-15-16(22)
InchiKey:	IJNHEFHRRKZQBBDK-UHFFFAOYSA-N
Formula:	C21H30Cl2O4
SMILES:	CCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1cc(Cl)ccc1Cl
Mol. weight [g/mol]:	417.37

## Physical Properties

Property code	Value	Unit	Source
gf	-269.77	kJ/mol	Joback Method
hf	-793.01	kJ/mol	Joback Method
hfus	49.96	kJ/mol	Joback Method
hvap	91.73	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	6.609		Crippen Method
mcvol	322.350	ml/mol	McGowan Method
pc	1192.35	kPa	Joback Method
rinpol	2609.00		NIST Webbook
rinpol	2609.00		NIST Webbook
tb	940.73	K	Joback Method
tc	1157.76	K	Joback Method
tf	584.47	K	Joback Method
vc	1.238	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	988.86	J/molxK	940.73	Joback Method
cpg	1047.56	J/molxK	1121.59	Joback Method
cpg	1037.98	J/molxK	1085.42	Joback Method
cpg	1027.37	J/molxK	1049.25	Joback Method
cpg	1015.68	J/molxK	1013.07	Joback Method
cpg	1002.86	J/molxK	976.90	Joback Method
cpg	1056.16	J/molxK	1157.76	Joback Method
dvisc	0.0000271	Paxs	940.73	Joback Method

dvisc	0.0000349	Paxs	881.35	Joback Method
dvisc	0.0000466	Paxs	821.98	Joback Method
dvisc	0.0000651	Paxs	762.60	Joback Method
dvisc	0.0000964	Paxs	703.22	Joback Method
dvisc	0.0001533	Paxs	643.85	Joback Method
dvisc	0.0002679	Paxs	584.47	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=U363687&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U363687&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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