

# Diethylmalonic acid, 2-chlorophenyl decyl ester

Inchi:	InChI=1S/C23H35ClO4/c1-4-7-8-9-10-11-12-15-18-27-21(25)23(5-2,6-3)22(26)28-20-17-
InchiKey:	QGMCJYSPEQTPNN-UHFFFAOYSA-N
Formula:	C23H35ClO4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1Cl
Mol. weight [g/mol]:	410.98

## Physical Properties

Property code	Value	Unit	Source
gf	-231.37	kJ/mol	Joback Method
hf	-807.08	kJ/mol	Joback Method
hfus	51.33	kJ/mol	Joback Method
hvap	91.13	kJ/mol	Joback Method
log10ws	-7.37		Crippen Method
logp	6.736		Crippen Method
mvol	338.290	ml/mol	McGowan Method
pc	1084.92	kPa	Joback Method
rinpol	2655.00		NIST Webbook
rinpol	2655.00		NIST Webbook
tb	944.08	K	Joback Method
tc	1158.58	K	Joback Method
tf	564.57	K	Joback Method
vc	1.302	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1085.19	J/molxK	944.08	Joback Method
cpg	1151.60	J/molxK	1122.83	Joback Method
cpg	1140.58	J/molxK	1087.08	Joback Method
cpg	1128.49	J/molxK	1051.33	Joback Method
cpg	1115.26	J/molxK	1015.58	Joback Method
cpg	1100.85	J/molxK	979.83	Joback Method
cpg	1161.61	J/molxK	1158.58	Joback Method
dvisc	0.0000232	Paxs	944.08	Joback Method

dvisc	0.0000305	Paxs	880.83	Joback Method
dvisc	0.0000419	Paxs	817.58	Joback Method
dvisc	0.0000606	Paxs	754.32	Joback Method
dvisc	0.0000939	Paxs	691.07	Joback Method
dvisc	0.0001588	Paxs	627.82	Joback Method
dvisc	0.0003023	Paxs	564.57	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=U369622&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369622&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</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>log<sub>p</sub>:</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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