

# Diethylmalonic acid, decyl 3,5-dichlorophenyl ester

Inchi:	InChI=1S/C23H34Cl2O4/c1-4-7-8-9-10-11-12-13-14-28-21(26)23(5-2,6-3)22(27)29-20-16
InchiKey:	DRNWBPYRXBATRX-UHFFFAOYSA-N
Formula:	C23H34Cl2O4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	445.42

## Physical Properties

Property code	Value	Unit	Source
gf	-252.93	kJ/mol	Joback Method
hf	-834.29	kJ/mol	Joback Method
hfus	55.14	kJ/mol	Joback Method
hvap	96.18	kJ/mol	Joback Method
log10ws	-8.06		Crippen Method
logp	7.389		Crippen Method
mvol	350.530	ml/mol	McGowan Method
pc	1048.69	kPa	Joback Method
rinpol	2725.00		NIST Webbook
rinpol	2725.00		NIST Webbook
tb	986.49	K	Joback Method
tc	1208.86	K	Joback Method
tf	607.01	K	Joback Method
vc	1.351	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1108.95	J/molxK	986.49	Joback Method
cpg	1123.37	J/molxK	1023.55	Joback Method
cpg	1136.52	J/molxK	1060.61	Joback Method
cpg	1148.46	J/molxK	1097.67	Joback Method
cpg	1159.26	J/molxK	1134.74	Joback Method
cpg	1168.97	J/molxK	1171.80	Joback Method
cpg	1177.65	J/molxK	1208.86	Joback Method
dvisc	0.0002092	Paxs	607.01	Joback Method

dvisc	0.0001172	Paxs	670.26	Joback Method
dvisc	0.0000726	Paxs	733.50	Joback Method
dvisc	0.0000485	Paxs	796.75	Joback Method
dvisc	0.0000344	Paxs	860.00	Joback Method
dvisc	0.0000255	Paxs	923.24	Joback Method
dvisc	0.0000197	Paxs	986.49	Joback Method

## Sources

<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=U370444&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370444&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>

## 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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