

# Diethylmalonic acid, 2,6-dichlorophenyl tetradecyl ester

Inchi:	InChI=1S/C27H42Cl2O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-21-32-25(30)27(5-2,6-3)26
InchiKey:	YCYKMPCXDQGNCH-UHFFFAOYSA-N
Formula:	C27H42Cl2O4
SMILES:	CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(Cl)cccc1Cl
Mol. weight [g/mol]:	501.53

## Physical Properties

Property code	Value	Unit	Source
gf	-219.25	kJ/mol	Joback Method
hf	-916.85	kJ/mol	Joback Method
hfus	65.50	kJ/mol	Joback Method
hvap	105.08	kJ/mol	Joback Method
log10ws	-9.73		Crippen Method
logp	8.950		Crippen Method
mcvol	406.890	ml/mol	McGowan Method
pc	829.55	kPa	Joback Method
rinpol	3125.00		NIST Webbook
rinpol	3125.00		NIST Webbook
tb	1078.01	K	Joback Method
tc	1323.54	K	Joback Method
tf	652.09	K	Joback Method
vc	1.575	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1355.04	J/molxK	1078.01	Joback Method
cpg	1418.34	J/molxK	1282.61	Joback Method
cpg	1408.37	J/molxK	1241.69	Joback Method
cpg	1397.16	J/molxK	1200.77	Joback Method
cpg	1384.60	J/molxK	1159.85	Joback Method
cpg	1370.60	J/molxK	1118.93	Joback Method
cpg	1427.16	J/molxK	1323.54	Joback Method
dvisc	0.0000103	Paxs	1078.01	Joback Method

dvisc	0.0000135	Paxs	1007.02	Joback Method
dvisc	0.0000184	Paxs	936.04	Joback Method
dvisc	0.0000263	Paxs	865.05	Joback Method
dvisc	0.0000402	Paxs	794.06	Joback Method
dvisc	0.0000668	Paxs	723.08	Joback Method
dvisc	0.0001238	Paxs	652.09	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=U369941&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369941&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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