

# Diethylmalonic acid, 2-chlorophenyl tetradecyl ester

Inchi:	InChI=1S/C27H43ClO4/c1-4-7-8-9-10-11-12-13-14-15-16-19-22-31-25(29)27(5-2,6-3)26
InchiKey:	VIVOIQNKDORXNG-UHFFFAOYSA-N
Formula:	C27H43ClO4
SMILES:	CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1Cl
Mol. weight [g/mol]:	467.08

## Physical Properties

Property code	Value	Unit	Source
gf	-197.69	kJ/mol	Joback Method
hf	-889.64	kJ/mol	Joback Method
hfus	61.69	kJ/mol	Joback Method
hvap	100.03	kJ/mol	Joback Method
log10ws	-9.04		Crippen Method
logp	8.296		Crippen Method
mvol	394.650	ml/mol	McGowan Method
pc	854.96	kPa	Joback Method
rinpol	3086.00		NIST Webbook
rinpol	3086.00		NIST Webbook
tb	1035.60	K	Joback Method
tc	1269.41	K	Joback Method
tf	609.65	K	Joback Method
vc	1.526	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1332.20	J/molxK	1035.60	Joback Method
cpg	1402.08	J/molxK	1230.44	Joback Method
cpg	1390.71	J/molxK	1191.47	Joback Method
cpg	1378.13	J/molxK	1152.50	Joback Method
cpg	1364.25	J/molxK	1113.54	Joback Method
cpg	1348.97	J/molxK	1074.57	Joback Method
cpg	1412.33	J/molxK	1269.41	Joback Method
dvisc	0.0000122	Paxs	1035.60	Joback Method

dvisc	0.0000162	Paxs	964.61	Joback Method
dvisc	0.0000225	Paxs	893.62	Joback Method
dvisc	0.0000330	Paxs	822.62	Joback Method
dvisc	0.0000522	Paxs	751.63	Joback Method
dvisc	0.0000907	Paxs	680.64	Joback Method
dvisc	0.0001793	Paxs	609.65	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=U369624&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369624&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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