

# Phthalic acid, 2-(3-chlorophenyl)ethyl tridecyl ester

Inchi:	InChI=1S/C29H39ClO4/c1-2-3-4-5-6-7-8-9-10-11-14-21-33-28(31)26-18-12-13-19-27(26)
InchiKey:	KREOLZKJAOMQSD-UHFFFAOYSA-N
Formula:	C29H39ClO4
SMILES:	CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCCc1cccc(Cl)c1
Mol. weight [g/mol]:	487.07

## Physical Properties

Property code	Value	Unit	Source
gf	-80.91	kJ/mol	Joback Method
hf	-697.11	kJ/mol	Joback Method
hfus	67.94	kJ/mol	Joback Method
hvap	108.72	kJ/mol	Joback Method
log10ws	-9.70		Crippen Method
logp	8.207		Crippen Method
mcvol	399.070	ml/mol	McGowan Method
pc	909.98	kPa	Joback Method
rinpol	3610.00		NIST Webbook
tb	1116.25	K	Joback Method
tc	1369.17	K	Joback Method
tf	668.71	K	Joback Method
vc	1.540	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1342.53	J/molxK	1116.25	Joback Method
cpg	1393.22	J/molxK	1327.01	Joback Method
cpg	1386.18	J/molxK	1284.86	Joback Method
cpg	1377.69	J/molxK	1242.71	Joback Method
cpg	1367.65	J/molxK	1200.56	Joback Method
cpg	1355.96	J/molxK	1158.40	Joback Method
cpg	1398.90	J/molxK	1369.17	Joback Method
dvisc	0.0000128	Paxs	1116.25	Joback Method
dvisc	0.0000164	Paxs	1041.66	Joback Method

dvisc	0.0000220	Paxs	967.07	Joback Method
dvisc	0.0000308	Paxs	892.48	Joback Method
dvisc	0.0000459	Paxs	817.89	Joback Method
dvisc	0.0000743	Paxs	743.30	Joback Method
dvisc	0.0001336	Paxs	668.71	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U377863&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377863&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.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>

## 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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