

# cis-Cyclohex-4-en-1,2-dicarboxylic acid, 4-chloro-3-methylphenyl nonyl ester

Inchi:	InChI=1S/C24H33ClO4/c1-3-4-5-6-7-8-11-16-28-23(26)20-12-9-10-13-21(20)24(27)29-19
InchiKey:	FZXYZPZKLAQFY-UHFFFAOYSA-N
Formula:	C24H33ClO4
SMILES:	CCCCCCCCCOC(=O)C1CC=CCC1C(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]:	420.97

## Physical Properties

Property code	Value	Unit	Source
gf	-188.72	kJ/mol	Joback Method
hf	-738.68	kJ/mol	Joback Method
hfus	55.08	kJ/mol	Joback Method
hvap	95.73	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	6.430		Crippen Method
mcvol	337.220	ml/mol	McGowan Method
pc	1142.89	kPa	Joback Method
rinsol	3010.00		NIST Webbook
tb	989.21	K	Joback Method
tc	1215.52	K	Joback Method
tf	589.84	K	Joback Method
vc	1.286	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1112.31	J/molxK	989.21	Joback Method
cpg	1126.86	J/molxK	1026.93	Joback Method
cpg	1139.73	J/molxK	1064.65	Joback Method
cpg	1150.94	J/molxK	1102.37	Joback Method
cpg	1160.55	J/molxK	1140.09	Joback Method
cpg	1168.59	J/molxK	1177.80	Joback Method
cpg	1175.09	J/molxK	1215.52	Joback Method
dvisc	0.0003579	Paxs	589.84	Joback Method
dvisc	0.0002068	Paxs	656.40	Joback Method

dvisc	0.0001322	Paxs	722.96	Joback Method
dvisc	0.0000911	Paxs	789.52	Joback Method
dvisc	0.0000666	Paxs	856.09	Joback Method
dvisc	0.0000509	Paxs	922.65	Joback Method
dvisc	0.0000403	Paxs	989.21	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=U382654&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382654&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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