

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

<b>Inchi:</b>	InChI=1S/C18H21ClO4/c1-3-10-22-17(20)14-6-4-5-7-15(14)18(21)23-13-8-9-16(19)12(2)
<b>InchiKey:</b>	WPIMLPDLSPTCT-UHFFFAOYSA-N
<b>Formula:</b>	C18H21ClO4
<b>SMILES:</b>	CCCOC(=O)C1CC=CCC1C(=O)Oc1ccc(Cl)c(C)c1
<b>Mol. weight [g/mol]:</b>	336.81

## Physical Properties

Property code	Value	Unit	Source
gf	-239.24	kJ/mol	Joback Method
hf	-614.84	kJ/mol	Joback Method
hfus	39.54	kJ/mol	Joback Method
hvap	82.37	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.089		Crippen Method
mcvol	252.680	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
rinpol	2424.00		NIST Webbook
tb	851.93	K	Joback Method
tc	1080.38	K	Joback Method
tf	522.22	K	Joback Method
vc	0.951	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.13	J/molxK	851.93	Joback Method
cpg	772.08	J/molxK	890.00	Joback Method
cpg	785.57	J/molxK	928.08	Joback Method
cpg	797.60	J/molxK	966.15	Joback Method
cpg	808.21	J/molxK	1004.23	Joback Method
cpg	817.40	J/molxK	1042.30	Joback Method
cpg	825.18	J/molxK	1080.38	Joback Method
dvisc	0.0006452	Paxs	522.22	Joback Method
dvisc	0.0003998	Paxs	577.17	Joback Method

dvisc	0.0002692	Paxs	632.12	Joback Method
dvisc	0.0001932	Paxs	687.08	Joback Method
dvisc	0.0001456	Paxs	742.03	Joback Method
dvisc	0.0001140	Paxs	796.98	Joback Method
dvisc	0.0000922	Paxs	851.93	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=U382646&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382646&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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