

# Sebacic acid, 2-chloro-5-methylphenyl hexyl ester

Inchi:	InChI=1S/C23H35ClO4/c1-3-4-5-12-17-27-22(25)13-10-8-6-7-9-11-14-23(26)28-21-18-19
InchiKey:	BDXBIVTVGDBXCZ-UHFFFAOYSA-N
Formula:	C23H35ClO4
SMILES:	CCCCCOC(=O)CCCCCCCC(=O)Oc1cc(C)ccc1Cl
Mol. weight [g/mol]:	410.98

## Physical Properties

Property code	Value	Unit	Source
gf	-243.84	kJ/mol	Joback Method
hf	-809.80	kJ/mol	Joback Method
hfus	58.36	kJ/mol	Joback Method
hvap	93.09	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	6.798		Crippen Method
mvol	338.290	ml/mol	McGowan Method
pc	1061.02	kPa	Joback Method
rinpol	2995.00		NIST Webbook
tb	952.29	K	Joback Method
tc	1166.50	K	Joback Method
tf	574.67	K	Joback Method
vc	1.312	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1084.19	J/molxK	952.29	Joback Method
cpg	1099.71	J/molxK	987.99	Joback Method
cpg	1113.87	J/molxK	1023.69	Joback Method
cpg	1126.72	J/molxK	1059.39	Joback Method
cpg	1138.27	J/molxK	1095.10	Joback Method
cpg	1148.57	J/molxK	1130.80	Joback Method
cpg	1157.64	J/molxK	1166.50	Joback Method
dvisc	0.0003047	Paxs	574.67	Joback Method
dvisc	0.0001724	Paxs	637.61	Joback Method

dvisc	0.0001081	Paxs	700.54	Joback Method
dvisc	0.0000732	Paxs	763.48	Joback Method
dvisc	0.0000526	Paxs	826.42	Joback Method
dvisc	0.0000396	Paxs	889.35	Joback Method
dvisc	0.0000309	Paxs	952.29	Joback Method

## Sources

<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=U355304&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355304&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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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