

# Sebacic acid, 2-chlorophenyl hexyl ester

**Inchi:** InChI=1S/C22H33ClO4/c1-2-3-4-13-18-26-21(24)16-9-7-5-6-8-10-17-22(25)27-20-15-12  
**InchiKey:** CSKGWFNYQZXJBY-UHFFFAOYSA-N  
**Formula:** C22H33ClO4  
**SMILES:** CCCCCCOC(=O)CCCCCCCC(=O)Oc1ccccc1Cl  
**Mol. weight [g/mol]:** 396.95

## Physical Properties

Property code	Value	Unit	Source
gf	-242.63	kJ/mol	Joback Method
hf	-777.69	kJ/mol	Joback Method
hfus	56.16	kJ/mol	Joback Method
hvap	90.20	kJ/mol	Joback Method
log10ws	-7.19		Crippen Method
logp	6.490		Crippen Method
mvol	324.200	ml/mol	McGowan Method
pc	1142.12	kPa	Joback Method
rinpol	2923.00		NIST Webbook
rinpol	2923.00		NIST Webbook
tb	924.43	K	Joback Method
tc	1134.12	K	Joback Method
tf	550.88	K	Joback Method
vc	1.256	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.36	J/molxK	924.43	Joback Method
cpg	1039.76	J/molxK	959.38	Joback Method
cpg	1053.89	J/molxK	994.33	Joback Method
cpg	1066.80	J/molxK	1029.27	Joback Method
cpg	1078.52	J/molxK	1064.22	Joback Method
cpg	1089.07	J/molxK	1099.17	Joback Method
cpg	1098.50	J/molxK	1134.12	Joback Method
dvisc	0.0003880	Paxs	550.88	Joback Method

dvisc	0.0002123	Paxs	613.14	Joback Method
dvisc	0.0001298	Paxs	675.40	Joback Method
dvisc	0.0000862	Paxs	737.65	Joback Method
dvisc	0.0000611	Paxs	799.91	Joback Method
dvisc	0.0000454	Paxs	862.17	Joback Method
dvisc	0.0000352	Paxs	924.43	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=U354431&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354431&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>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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