

# Sebacic acid, 2-(2-chlorophenoxy)ethyl hexyl ester

Inchi:	InChI=1S/C24H37ClO5/c1-2-3-4-13-18-29-23(26)16-9-7-5-6-8-10-17-24(27)30-20-19-28
InchiKey:	RKDFDCIPMJQMXX-UHFFFAOYSA-N
Formula:	C24H37ClO5
SMILES:	CCCCCOC(=O)CCCCCCCC(=O)OCCOc1ccccc1Cl
Mol. weight [g/mol]:	441.00

## Physical Properties

Property code	Value	Unit	Source
gf	-330.79	kJ/mol	Joback Method
hf	-951.19	kJ/mol	Joback Method
hfus	62.53	kJ/mol	Joback Method
hvap	97.06	kJ/mol	Joback Method
log10ws	-7.12		Crippen Method
logp	6.506		Crippen Method
mvol	358.250	ml/mol	McGowan Method
pc	996.39	kPa	Joback Method
rinpol	3033.00		NIST Webbook
tb	992.61	K	Joback Method
tc	1215.50	K	Joback Method
tf	595.65	K	Joback Method
vc	1.387	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1174.62	J/molxK	992.61	Joback Method
cpg	1234.29	J/molxK	1178.35	Joback Method
cpg	1225.45	J/molxK	1141.20	Joback Method
cpg	1215.09	J/molxK	1104.06	Joback Method
cpg	1203.19	J/molxK	1066.91	Joback Method
cpg	1189.71	J/molxK	1029.76	Joback Method
cpg	1241.66	J/molxK	1215.50	Joback Method
dvisc	0.0000191	Paxs	992.61	Joback Method
dvisc	0.0000248	Paxs	926.45	Joback Method

dvisc	0.0000333	Paxs	860.29	Joback Method
dvisc	0.0000472	Paxs	794.13	Joback Method
dvisc	0.0000711	Paxs	727.97	Joback Method
dvisc	0.0001162	Paxs	661.81	Joback Method
dvisc	0.0002121	Paxs	595.65	Joback Method

## Sources

<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=U416775&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416775&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>

## 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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