

# Sebacic acid, isohexyl 3,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C22H31Cl3O4/c1-16(2)10-9-13-28-20(26)11-7-5-3-4-6-8-12-21(27)29-17-14-18
InchiKey:	XBMIPTYCIHKWND-UHFFFAOYSA-N
Formula:	C22H31Cl3O4
SMILES:	CC(C)CCCOC(=O)CCCCCCCC(=O)Oc1cc(Cl)c(Cl)c(Cl)c1
Mol. weight [g/mol]:	465.84

## Physical Properties

Property code	Value	Unit	Source
gf	-288.19	kJ/mol	Joback Method
hf	-837.39	kJ/mol	Joback Method
hfus	60.25	kJ/mol	Joback Method
hvap	99.91	kJ/mol	Joback Method
log10ws	-8.32		Crippen Method
logp	7.652		Crippen Method
mvol	348.680	ml/mol	McGowan Method
pc	1071.46	kPa	Joback Method
rinpol	3242.00		NIST Webbook
rinpol	3242.00		NIST Webbook
tb	1008.81	K	Joback Method
tc	1235.42	K	Joback Method
tf	620.76	K	Joback Method
vc	1.349	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1070.25	J/molxK	1008.81	Joback Method
cpg	1120.13	J/molxK	1197.65	Joback Method
cpg	1112.84	J/molxK	1159.88	Joback Method
cpg	1104.24	J/molxK	1122.12	Joback Method
cpg	1094.29	J/molxK	1084.35	Joback Method
cpg	1082.97	J/molxK	1046.58	Joback Method
cpg	1126.15	J/molxK	1235.42	Joback Method
dvisc	0.0000237	Paxs	1008.81	Joback Method

dvisc	0.0000302	Paxs	944.13	Joback Method
dvisc	0.0000398	Paxs	879.46	Joback Method
dvisc	0.0000548	Paxs	814.78	Joback Method
dvisc	0.0000798	Paxs	750.11	Joback Method
dvisc	0.0001248	Paxs	685.43	Joback Method
dvisc	0.0002140	Paxs	620.76	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=U355224&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355224&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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