

# Sebacic acid, di(3-chlorophenyl) ester

<b>Inchi:</b>	InChI=1S/C22H24Cl2O4/c23-17-9-7-11-19(15-17)27-21(25)13-5-3-1-2-4-6-14-22(26)28-2
<b>InchiKey:</b>	NEFVXKLD SURJDH-UHFFFAOYSA-N
<b>Formula:</b>	C22H24Cl2O4
<b>SMILES:</b>	O=C(CCCCCCCC(=O)Oc1cccc(Cl)c1)Oc1cccc(Cl)c1
<b>Mol. weight [g/mol]:</b>	423.33

## Physical Properties

Property code	Value	Unit	Source
gf	-151.78	kJ/mol	Joback Method
hf	-568.37	kJ/mol	Joback Method
hfus	54.01	kJ/mol	Joback Method
hvap	97.52	kJ/mol	Joback Method
log10ws	-7.63		Crippen Method
logp	6.625		Crippen Method
mvol	312.680	ml/mol	McGowan Method
pc	1392.29	kPa	Joback Method
rinpol	3348.00		NIST Webbook
tb	993.52	K	Joback Method
tc	1225.45	K	Joback Method
tf	619.74	K	Joback Method
vc	1.198	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.76	J/molxK	993.52	Joback Method
cpg	952.26	J/molxK	1032.18	Joback Method
cpg	962.43	J/molxK	1070.83	Joback Method
cpg	971.34	J/molxK	1109.49	Joback Method
cpg	979.02	J/molxK	1148.14	Joback Method
cpg	985.52	J/molxK	1186.80	Joback Method
cpg	990.90	J/molxK	1225.45	Joback Method
dvisc	0.0002519	Paxs	619.74	Joback Method
dvisc	0.0001520	Paxs	682.04	Joback Method

dvisc	0.0000999	Paxs	744.33	Joback Method
dvisc	0.0000700	Paxs	806.63	Joback Method
dvisc	0.0000516	Paxs	868.93	Joback Method
dvisc	0.0000397	Paxs	931.22	Joback Method
dvisc	0.0000315	Paxs	993.52	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=U354871&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354871&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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