

# Sebacic acid, heptyl 2,3,6-trichlorophenyl ester

Inchi:	InChI=1S/C23H33Cl3O4/c1-2-3-4-9-12-17-29-20(27)13-10-7-5-6-8-11-14-21(28)30-23-19
InchiKey:	NOMSBMXNHIJCRM-UHFFFAOYSA-N
Formula:	C23H33Cl3O4
SMILES:	CCCCCCCC(=O)CCCCCCCC(=O)Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]:	479.87

## Physical Properties

Property code	Value	Unit	Source
gf	-277.33	kJ/mol	Joback Method
hf	-852.75	kJ/mol	Joback Method
hfus	66.37	kJ/mol	Joback Method
hvap	102.52	kJ/mol	Joback Method
log10ws	-8.98		Crippen Method
logp	8.187		Crippen Method
mcvol	362.770	ml/mol	McGowan Method
pc	1002.08	kPa	Joback Method
rinpol	3315.00		NIST Webbook
tb	1032.13	K	Joback Method
tc	1263.80	K	Joback Method
tf	647.03	K	Joback Method
vc	1.411	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1130.08	J/molxK	1032.13	Joback Method
cpg	1143.05	J/molxK	1070.74	Joback Method
cpg	1154.54	J/molxK	1109.35	Joback Method
cpg	1164.59	J/molxK	1147.97	Joback Method
cpg	1173.23	J/molxK	1186.58	Joback Method
cpg	1180.50	J/molxK	1225.19	Joback Method
cpg	1186.45	J/molxK	1263.80	Joback Method
dvisc	0.0001787	Paxs	647.03	Joback Method
dvisc	0.0001081	Paxs	711.21	Joback Method

dvisc	0.0000710	Paxs	775.40	Joback Method
dvisc	0.0000498	Paxs	839.58	Joback Method
dvisc	0.0000367	Paxs	903.76	Joback Method
dvisc	0.0000282	Paxs	967.95	Joback Method
dvisc	0.0000223	Paxs	1032.13	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U355266&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355266&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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