

# Sebacic acid, pentyl 2,4,6-trichlorophenyl ester

<b>Inchi:</b>	InChI=1S/C21H29Cl3O4/c1-2-3-10-13-27-19(25)11-8-6-4-5-7-9-12-20(26)28-21-17(23)14
<b>InchiKey:</b>	CKHQSKQYJCMVAF-UHFFFAOYSA-N
<b>Formula:</b>	C21H29Cl3O4
<b>SMILES:</b>	CCCCCOC(=O)CCCCCCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	451.81

## Physical Properties

Property code	Value	Unit	Source
gf	-294.17	kJ/mol	Joback Method
hf	-811.47	kJ/mol	Joback Method
hfus	61.18	kJ/mol	Joback Method
hvap	98.07	kJ/mol	Joback Method
log10ws	-8.14		Crippen Method
logp	7.406		Crippen Method
mvol	334.590	ml/mol	McGowan Method
pc	1135.96	kPa	Joback Method
rinpol	3046.00		NIST Webbook
rinpol	3046.00		NIST Webbook
tb	986.37	K	Joback Method
tc	1208.66	K	Joback Method
tf	624.49	K	Joback Method
vc	1.298	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1010.15	J/molxK	986.37	Joback Method
cpg	1022.76	J/molxK	1023.42	Joback Method
cpg	1034.05	J/molxK	1060.47	Joback Method
cpg	1044.06	J/molxK	1097.52	Joback Method
cpg	1052.81	J/molxK	1134.57	Joback Method
cpg	1060.33	J/molxK	1171.62	Joback Method
cpg	1066.65	J/molxK	1208.66	Joback Method
dvisc	0.0002266	Paxs	624.49	Joback Method

dvisc	0.0001399	Paxs	684.80	Joback Method
dvisc	0.0000934	Paxs	745.12	Joback Method
dvisc	0.0000663	Paxs	805.43	Joback Method
dvisc	0.0000493	Paxs	865.74	Joback Method
dvisc	0.0000381	Paxs	926.06	Joback Method
dvisc	0.0000304	Paxs	986.37	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=U355078&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355078&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>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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