

# Sebacic acid, octyl 2,4,5-trichlorophenyl ester

**Inchi:** InChI=1S/C24H35Cl3O4/c1-2-3-4-5-10-13-16-30-23(28)14-11-8-6-7-9-12-15-24(29)31-22  
**InchiKey:** SEHAVLPGPNPEPY-UHFFFAOYSA-N  
**Formula:** C24H35Cl3O4  
**SMILES:** CCCCCCOC(=O)CCCCCCCC(=O)Oc1cc(Cl)c(Cl)cc1Cl  
**Mol. weight [g/mol]:** 493.89

## Physical Properties

Property code	Value	Unit	Source
gf	-268.91	kJ/mol	Joback Method
hf	-873.39	kJ/mol	Joback Method
hfus	68.95	kJ/mol	Joback Method
hvap	104.75	kJ/mol	Joback Method
log10ws	-9.40		Crippen Method
logp	8.577		Crippen Method
mvol	376.860	ml/mol	McGowan Method
pc	943.84	kPa	Joback Method
rinpol	3412.00		NIST Webbook
rinpol	3412.00		NIST Webbook
tb	1055.01	K	Joback Method
tc	1293.03	K	Joback Method
tf	658.30	K	Joback Method
vc	1.466	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1190.69	J/molxK	1055.01	Joback Method
cpg	1203.86	J/molxK	1094.68	Joback Method
cpg	1215.43	J/molxK	1134.35	Joback Method
cpg	1225.47	J/molxK	1174.02	Joback Method
cpg	1234.01	J/molxK	1213.69	Joback Method
cpg	1241.10	J/molxK	1253.36	Joback Method
cpg	1246.79	J/molxK	1293.03	Joback Method
dvisc	0.0001581	Paxs	658.30	Joback Method

dvisc	0.0000946	Paxs	724.42	Joback Method
dvisc	0.0000617	Paxs	790.54	Joback Method
dvisc	0.0000430	Paxs	856.65	Joback Method
dvisc	0.0000316	Paxs	922.77	Joback Method
dvisc	0.0000241	Paxs	988.89	Joback Method
dvisc	0.0000191	Paxs	1055.01	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U355198&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355198&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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