

# Sebacic acid, pentyl 2,2,2-trichloroethyl ester

<b>Inchi:</b>	InChI=1S/C17H29Cl3O4/c1-2-3-10-13-23-15(21)11-8-6-4-5-7-9-12-16(22)24-14-17(18,19)
<b>InchiKey:</b>	OHOLQHOFSHVAHP-UHFFFAOYSA-N
<b>Formula:</b>	C17H29Cl3O4
<b>SMILES:</b>	CCCCCOC(=O)CCCCCCCCC(=O)OCC(Cl)(Cl)Cl
<b>Mol. weight [g/mol]:</b>	403.77

## Physical Properties

Property code	Value	Unit	Source
gf	-408.53	kJ/mol	Joback Method
hf	-939.78	kJ/mol	Joback Method
hfus	50.54	kJ/mol	Joback Method
hvap	83.61	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	5.754		Crippen Method
mcvol	301.990	ml/mol	McGowan Method
pc	1231.15	kPa	Joback Method
rinpol	2517.00		NIST Webbook
rinpol	2517.00		NIST Webbook
tb	850.00	K	Joback Method
tc	1047.84	K	Joback Method
tf	517.85	K	Joback Method
vc	1.171	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.37	J/molxK	850.00	Joback Method
cpg	942.37	J/molxK	1014.86	Joback Method
cpg	931.76	J/molxK	981.89	Joback Method
cpg	920.29	J/molxK	948.92	Joback Method
cpg	907.93	J/molxK	915.95	Joback Method
cpg	894.63	J/molxK	882.97	Joback Method
cpg	952.15	J/molxK	1047.84	Joback Method
dvisc	0.0000406	Paxs	850.00	Joback Method

dvisc	0.0000537	Paxs	794.64	Joback Method
dvisc	0.0000740	Paxs	739.28	Joback Method
dvisc	0.0001073	Paxs	683.92	Joback Method
dvisc	0.0001663	Paxs	628.57	Joback Method
dvisc	0.0002806	Paxs	573.21	Joback Method
dvisc	0.0005291	Paxs	517.85	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=U355313&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355313&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>

## 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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