

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

**Inchi:** InChI=1S/C19H33Cl3O4/c1-2-3-4-9-12-15-25-17(23)13-10-7-5-6-8-11-14-18(24)26-16-19  
**InchiKey:** IWJFYUCYOYVGKN-UHFFFAOYSA-N  
**Formula:** C19H33Cl3O4  
**SMILES:** CCCCCCOC(=O)CCCCCCCC(=O)OCC(Cl)(Cl)Cl  
**Mol. weight [g/mol]:** 431.82

## Physical Properties

Property code	Value	Unit	Source
gf	-391.69	kJ/mol	Joback Method
hf	-981.06	kJ/mol	Joback Method
hfus	55.72	kJ/mol	Joback Method
hvap	88.06	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	6.534		Crippen Method
mvol	330.170	ml/mol	McGowan Method
pc	1080.64	kPa	Joback Method
rinpol	2718.00		NIST Webbook
rinpol	2718.00		NIST Webbook
tb	895.76	K	Joback Method
tc	1098.51	K	Joback Method
tf	540.39	K	Joback Method
vc	1.284	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.08	J/molxK	895.76	Joback Method
cpg	1013.04	J/molxK	929.55	Joback Method
cpg	1026.95	J/molxK	963.34	Joback Method
cpg	1039.83	J/molxK	997.14	Joback Method
cpg	1051.74	J/molxK	1030.93	Joback Method
cpg	1062.71	J/molxK	1064.72	Joback Method
cpg	1072.80	J/molxK	1098.51	Joback Method
dvisc	0.0004095	Paxs	540.39	Joback Method

dvisc	0.0002124	Paxs	599.62	Joback Method
dvisc	0.0001240	Paxs	658.85	Joback Method
dvisc	0.0000791	Paxs	718.08	Joback Method
dvisc	0.0000540	Paxs	777.30	Joback Method
dvisc	0.0000390	Paxs	836.53	Joback Method
dvisc	0.0000293	Paxs	895.76	Joback Method

## Sources

<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=U355315&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355315&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

## 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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