

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

Inchi:	InChI=1S/C24H43Cl3O4/c1-2-3-4-5-6-7-8-11-14-17-20-30-22(28)18-15-12-9-10-13-16-19
InchiKey:	NFXYFERQSI AEGN-UHFFFAOYSA-N
Formula:	C24H43Cl3O4
SMILES:	CCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	501.95

## Physical Properties

Property code	Value	Unit	Source
gf	-349.59	kJ/mol	Joback Method
hf	-1084.26	kJ/mol	Joback Method
hfus	68.67	kJ/mol	Joback Method
hvap	99.19	kJ/mol	Joback Method
log10ws	-9.16		Crippen Method
logp	8.485		Crippen Method
mvol	400.620	ml/mol	McGowan Method
pc	806.16	kPa	Joback Method
rinpol	3228.00		NIST Webbook
rinpol	3228.00		NIST Webbook
tb	1010.16	K	Joback Method
tc	1241.73	K	Joback Method
tf	596.74	K	Joback Method
vc	1.563	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1303.59	J/molxK	1010.16	Joback Method
cpg	1375.71	J/molxK	1203.13	Joback Method
cpg	1363.82	J/molxK	1164.54	Joback Method
cpg	1350.75	J/molxK	1125.94	Joback Method
cpg	1336.41	J/molxK	1087.35	Joback Method
cpg	1320.72	J/molxK	1048.75	Joback Method
cpg	1386.50	J/molxK	1241.73	Joback Method
dvisc	0.0000128	Paxs	1010.16	Joback Method

dvisc	0.0000171	Paxs	941.26	Joback Method
dvisc	0.0000241	Paxs	872.35	Joback Method
dvisc	0.0000359	Paxs	803.45	Joback Method
dvisc	0.0000577	Paxs	734.55	Joback Method
dvisc	0.0001022	Paxs	665.64	Joback Method
dvisc	0.0002068	Paxs	596.74	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U355320&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355320&amp;Units=SI</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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