

# Sebacic acid, 2,2-dichloroethyl tridecyl ester

<b>Inchi:</b>	InChI=1S/C25H46Cl2O4/c1-2-3-4-5-6-7-8-9-12-15-18-21-30-24(28)19-16-13-10-11-14-17
<b>InchiKey:</b>	CIFOYKFDYAJUPH-UHFFFAOYSA-N
<b>Formula:</b>	C25H46Cl2O4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)CCCCCCCC(=O)OCC(Cl)Cl
<b>Mol. weight [g/mol]:</b>	481.54

## Physical Properties

Property code	Value	Unit	Source
gf	-334.52	kJ/mol	Joback Method
hf	-1085.69	kJ/mol	Joback Method
hfus	70.95	kJ/mol	Joback Method
hvap	97.94	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	8.308		Crippen Method
mvol	402.470	ml/mol	McGowan Method
pc	775.05	kPa	Joback Method
rinpol	3246.00		NIST Webbook
rinpol	3246.00		NIST Webbook
tb	998.40	K	Joback Method
tc	1230.91	K	Joback Method
tf	560.67	K	Joback Method
vc	1.575	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1340.42	J/molxK	998.40	Joback Method
cpg	1359.09	J/molxK	1037.15	Joback Method
cpg	1376.04	J/molxK	1075.90	Joback Method
cpg	1391.33	J/molxK	1114.66	Joback Method
cpg	1405.03	J/molxK	1153.41	Joback Method
cpg	1417.19	J/molxK	1192.16	Joback Method
cpg	1427.88	J/molxK	1230.91	Joback Method
dvisc	0.0003061	Paxs	560.67	Joback Method

dvisc	0.0001408	Paxs	633.62	Joback Method
dvisc	0.0000760	Paxs	706.58	Joback Method
dvisc	0.0000461	Paxs	779.53	Joback Method
dvisc	0.0000304	Paxs	852.49	Joback Method
dvisc	0.0000214	Paxs	925.44	Joback Method
dvisc	0.0000159	Paxs	998.40	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=U355476&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355476&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>
<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>

## 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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