

# Adipic acid, 2,2-dichloroethyl tridecyl ester

<b>Inchi:</b>	InChI=1S/C21H38Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-14-17-26-20(24)15-12-13-16-21(25)27
<b>InchiKey:</b>	DPSNXKATXBEHMW-UHFFFAOYSA-N
<b>Formula:</b>	C21H38Cl2O4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)CCCC(=O)OCC(Cl)Cl
<b>Mol. weight [g/mol]:</b>	425.43

## Physical Properties

Property code	Value	Unit	Source
gf	-368.20	kJ/mol	Joback Method
hf	-1003.13	kJ/mol	Joback Method
hfus	60.59	kJ/mol	Joback Method
hvap	89.03	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	6.748		Crippen Method
mvol	346.110	ml/mol	McGowan Method
pc	971.70	kPa	Joback Method
rinpol	2798.00		NIST Webbook
rinpol	2798.00		NIST Webbook
tb	906.88	K	Joback Method
tc	1110.28	K	Joback Method
tf	515.59	K	Joback Method
vc	1.351	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.61	J/molxK	906.88	Joback Method
cpg	1108.43	J/molxK	940.78	Joback Method
cpg	1124.01	J/molxK	974.68	Joback Method
cpg	1138.38	J/molxK	1008.58	Joback Method
cpg	1151.56	J/molxK	1042.48	Joback Method
cpg	1163.60	J/molxK	1076.38	Joback Method
cpg	1174.51	J/molxK	1110.28	Joback Method
dvisc	0.0005208	Paxs	515.59	Joback Method

dvisc	0.0002481	Paxs	580.80	Joback Method
dvisc	0.0001373	Paxs	646.02	Joback Method
dvisc	0.0000847	Paxs	711.23	Joback Method
dvisc	0.0000566	Paxs	776.45	Joback Method
dvisc	0.0000403	Paxs	841.66	Joback Method
dvisc	0.0000301	Paxs	906.88	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=U353587&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353587&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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