

# Adipic acid, 2,2-dichloroethyl pentadecyl ester

<b>Inchi:</b>	InChI=1S/C23H42Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-19-28-22(26)17-14-15-18-20
<b>InchiKey:</b>	QDFMQSCGUQMMII-UHFFFAOYSA-N
<b>Formula:</b>	C23H42Cl2O4
<b>SMILES:</b>	CCCCCCCCCCCCCOC(=O)CCCC(=O)OCC(Cl)Cl
<b>Mol. weight [g/mol]:</b>	453.48

## Physical Properties

Property code	Value	Unit	Source
gf	-351.36	kJ/mol	Joback Method
hf	-1044.41	kJ/mol	Joback Method
hfus	65.77	kJ/mol	Joback Method
hvap	93.49	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	7.528		Crippen Method
mvol	374.290	ml/mol	McGowan Method
pc	865.05	kPa	Joback Method
rinpol	3000.00		NIST Webbook
tb	952.64	K	Joback Method
tc	1168.33	K	Joback Method
tf	538.13	K	Joback Method
vc	1.464	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1215.05	J/molxK	952.64	Joback Method
cpg	1232.73	J/molxK	988.59	Joback Method
cpg	1248.97	J/molxK	1024.54	Joback Method
cpg	1263.80	J/molxK	1060.49	Joback Method
cpg	1277.27	J/molxK	1096.43	Joback Method
cpg	1289.41	J/molxK	1132.38	Joback Method
cpg	1300.28	J/molxK	1168.33	Joback Method
dvisc	0.0004012	Paxs	538.13	Joback Method
dvisc	0.0001877	Paxs	607.22	Joback Method

dvisc	0.0001026	Paxs	676.30	Joback Method
dvisc	0.0000627	Paxs	745.38	Joback Method
dvisc	0.0000416	Paxs	814.47	Joback Method
dvisc	0.0000295	Paxs	883.55	Joback Method
dvisc	0.0000220	Paxs	952.64	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=U353589&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353589&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>

## 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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