

# Adipic acid, 2,2-dichloroethyl octyl ester

<b>Inchi:</b>	InChI=1S/C16H28Cl2O4/c1-2-3-4-5-6-9-12-21-15(19)10-7-8-11-16(20)22-13-14(17)18/h
<b>InchiKey:</b>	FVTKGENJJVDTOL-UHFFFAOYSA-N
<b>Formula:</b>	C16H28Cl2O4
<b>SMILES:</b>	CCCCCCCCOC(=O)CCCCC(=O)OCC(Cl)Cl
<b>Mol. weight [g/mol]:</b>	355.30

## Physical Properties

Property code	Value	Unit	Source
gf	-410.30	kJ/mol	Joback Method
hf	-899.93	kJ/mol	Joback Method
hfus	47.64	kJ/mol	Joback Method
hvap	77.90	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.797		Crippen Method
mvol	275.660	ml/mol	McGowan Method
pc	1343.73	kPa	Joback Method
rinpol	2297.00		NIST Webbook
rinpol	2297.00		NIST Webbook
tb	792.48	K	Joback Method
tc	980.97	K	Joback Method
tf	459.24	K	Joback Method
vc	1.071	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.61	J/molxK	792.48	Joback Method
cpg	809.56	J/molxK	823.89	Joback Method
cpg	823.60	J/molxK	855.31	Joback Method
cpg	836.74	J/molxK	886.72	Joback Method
cpg	849.01	J/molxK	918.14	Joback Method
cpg	860.40	J/molxK	949.55	Joback Method
cpg	870.93	J/molxK	980.97	Joback Method
dvisc	0.0009489	Paxs	459.24	Joback Method

dvisc	0.0004763	Paxs	514.78	Joback Method
dvisc	0.0002734	Paxs	570.32	Joback Method
dvisc	0.0001732	Paxs	625.86	Joback Method
dvisc	0.0001182	Paxs	681.40	Joback Method
dvisc	0.0000854	Paxs	736.94	Joback Method
dvisc	0.0000646	Paxs	792.48	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=U353582&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353582&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.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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