

# Adipic acid, octyl 2,2,2-trichloroethyl ester

<b>Inchi:</b>	InChI=1S/C16H27Cl3O4/c1-2-3-4-5-6-9-12-22-14(20)10-7-8-11-15(21)23-13-16(17,18)19
<b>InchiKey:</b>	MOPKYJGIVGWDBI-UHFFFAOYSA-N
<b>Formula:</b>	C16H27Cl3O4
<b>SMILES:</b>	CCCCCCCCOC(=O)CCCCC(=O)OCC(Cl)(Cl)Cl
<b>Mol. weight [g/mol]:</b>	389.74

## Physical Properties

Property code	Value	Unit	Source
gf	-416.95	kJ/mol	Joback Method
hf	-919.14	kJ/mol	Joback Method
hfus	47.95	kJ/mol	Joback Method
hvap	81.38	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.364		Crippen Method
mvol	287.900	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	2366.00		NIST Webbook
rinpol	2366.00		NIST Webbook
tb	827.12	K	Joback Method
tc	1023.65	K	Joback Method
tf	506.58	K	Joback Method
vc	1.115	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.70	J/molxK	827.12	Joback Method
cpg	836.62	J/molxK	859.88	Joback Method
cpg	849.62	J/molxK	892.63	Joback Method
cpg	861.72	J/molxK	925.39	Joback Method
cpg	872.95	J/molxK	958.14	Joback Method
cpg	883.35	J/molxK	990.90	Joback Method
cpg	892.96	J/molxK	1023.65	Joback Method
dvisc	0.0005990	Paxs	506.58	Joback Method

dvisc	0.0003213	Paxs	560.00	Joback Method
dvisc	0.0001921	Paxs	613.43	Joback Method
dvisc	0.0001247	Paxs	666.85	Joback Method
dvisc	0.0000863	Paxs	720.27	Joback Method
dvisc	0.0000628	Paxs	773.70	Joback Method
dvisc	0.0000477	Paxs	827.12	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=U353480&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353480&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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