

# Adipic acid, ethyl 3,4,5-trichlorophenyl ester

<b>Inchi:</b>	InChI=1S/C14H15Cl3O4/c1-2-20-12(18)5-3-4-6-13(19)21-9-7-10(15)14(17)11(16)8-9/h7-
<b>InchiKey:</b>	JEUSXSJAJXPRRB-UHFFFAOYSA-N
<b>Formula:</b>	C14H15Cl3O4
<b>SMILES:</b>	CCOC(=O)CCCCC(=O)Oc1cc(Cl)c(Cl)c(Cl)c1
<b>Mol. weight [g/mol]:</b>	353.62

## Physical Properties

Property code	Value	Unit	Source
gf	-353.11	kJ/mol	Joback Method
hf	-666.99	kJ/mol	Joback Method
hfus	43.05	kJ/mol	Joback Method
hvap	82.49	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.676		Crippen Method
mcvol	235.960	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinsol	2414.00		NIST Webbook
tb	826.21	K	Joback Method
tc	1043.90	K	Joback Method
tf	545.60	K	Joback Method
vc	0.906	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.81	J/molxK	826.21	Joback Method
cpg	620.76	J/molxK	862.49	Joback Method
cpg	630.78	J/molxK	898.77	Joback Method
cpg	639.87	J/molxK	935.06	Joback Method
cpg	648.02	J/molxK	971.34	Joback Method
cpg	655.24	J/molxK	1007.62	Joback Method
cpg	661.54	J/molxK	1043.90	Joback Method
dvisc	0.0004707	Paxs	545.60	Joback Method
dvisc	0.0003158	Paxs	592.37	Joback Method

dvisc	0.0002246	Paxs	639.14	Joback Method
dvisc	0.0001673	Paxs	685.90	Joback Method
dvisc	0.0001294	Paxs	732.67	Joback Method
dvisc	0.0001033	Paxs	779.44	Joback Method
dvisc	0.0000845	Paxs	826.21	Joback Method

## Sources

<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=U353904&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353904&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>

## 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>mccvol:</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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