

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

<b>Inchi:</b>	InChI=1S/C15H17Cl3O4/c1-2-7-21-13(19)5-3-4-6-14(20)22-10-8-11(16)15(18)12(17)9-10
<b>InchiKey:</b>	PNPBBANVMWOHJL-UHFFFAOYSA-N
<b>Formula:</b>	C15H17Cl3O4
<b>SMILES:</b>	CCCOC(=O)CCCCC(=O)Oc1cc(Cl)c(Cl)c(Cl)c1
<b>Mol. weight [g/mol]:</b>	367.65

## Physical Properties

Property code	Value	Unit	Source
gf	-344.69	kJ/mol	Joback Method
hf	-687.63	kJ/mol	Joback Method
hfus	45.64	kJ/mol	Joback Method
hvap	84.71	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	5.066		Crippen Method
mcvol	250.050	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinsol	2517.00		NIST Webbook
tb	849.09	K	Joback Method
tc	1065.19	K	Joback Method
tf	556.87	K	Joback Method
vc	0.963	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.65	J/molxK	849.09	Joback Method
cpg	711.31	J/molxK	1029.18	Joback Method
cpg	703.92	J/molxK	993.16	Joback Method
cpg	695.56	J/molxK	957.14	Joback Method
cpg	686.23	J/molxK	921.12	Joback Method
cpg	675.93	J/molxK	885.11	Joback Method
cpg	717.74	J/molxK	1065.19	Joback Method
dvisc	0.0000735	Paxs	849.09	Joback Method
dvisc	0.0000902	Paxs	800.39	Joback Method

dvisc	0.0001137	Paxs	751.68	Joback Method
dvisc	0.0001478	Paxs	702.98	Joback Method
dvisc	0.0002000	Paxs	654.28	Joback Method
dvisc	0.0002840	Paxs	605.57	Joback Method
dvisc	0.0004288	Paxs	556.87	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=U353905&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353905&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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