

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

<b>Inchi:</b>	InChI=1S/C17H21Cl3O4/c1-2-3-6-9-23-15(21)7-4-5-8-16(22)24-12-10-13(18)17(20)14(19)
<b>InchiKey:</b>	ONMLPCQHQTDDP-UHFFFAOYSA-N
<b>Formula:</b>	C17H21Cl3O4
<b>SMILES:</b>	CCCCCOC(=O)CCCCC(=O)Oc1cc(Cl)c(Cl)c(Cl)c1
<b>Mol. weight [g/mol]:</b>	395.70

## Physical Properties

Property code	Value	Unit	Source
gf	-327.85	kJ/mol	Joback Method
hf	-728.91	kJ/mol	Joback Method
hfus	50.82	kJ/mol	Joback Method
hvap	89.16	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	5.846		Crippen Method
mcvol	278.230	ml/mol	McGowan Method
pc	1498.83	kPa	Joback Method
rinqol	2708.00		NIST Webbook
tb	894.85	K	Joback Method
tc	1109.82	K	Joback Method
tf	579.41	K	Joback Method
vc	1.075	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.95	J/molxK	894.85	Joback Method
cpg	788.76	J/molxK	930.68	Joback Method
cpg	799.50	J/molxK	966.51	Joback Method
cpg	809.18	J/molxK	1002.34	Joback Method
cpg	817.80	J/molxK	1038.17	Joback Method
cpg	825.39	J/molxK	1073.99	Joback Method
cpg	831.96	J/molxK	1109.82	Joback Method
dvisc	0.0003515	Paxs	579.41	Joback Method
dvisc	0.0002271	Paxs	631.98	Joback Method

dvisc	0.0001570	Paxs	684.56	Joback Method
dvisc	0.0001143	Paxs	737.13	Joback Method
dvisc	0.0000869	Paxs	789.70	Joback Method
dvisc	0.0000683	Paxs	842.28	Joback Method
dvisc	0.0000553	Paxs	894.85	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=U353908&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353908&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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