

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

<b>Inchi:</b>	InChI=1S/C19H25Cl3O4/c1-2-3-4-5-8-11-25-17(23)9-6-7-10-18(24)26-14-12-15(20)19(22)
<b>InchiKey:</b>	ZGPQRTBRZPSUHQ-UHFFFAOYSA-N
<b>Formula:</b>	C19H25Cl3O4
<b>SMILES:</b>	CCCCCCCOC(=O)CCCCC(=O)Oc1cc(Cl)c(Cl)c(Cl)c1
<b>Mol. weight [g/mol]:</b>	423.76

## Physical Properties

Property code	Value	Unit	Source
gf	-311.01	kJ/mol	Joback Method
hf	-770.19	kJ/mol	Joback Method
hfus	56.00	kJ/mol	Joback Method
hvap	93.62	kJ/mol	Joback Method
log10ws	-7.31		Crippen Method
logp	6.626		Crippen Method
mcvol	306.410	ml/mol	McGowan Method
pc	1298.60	kPa	Joback Method
rinqol	2914.00		NIST Webbook
tb	940.61	K	Joback Method
tc	1157.50	K	Joback Method
tf	601.95	K	Joback Method
vc	1.187	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.29	J/molxK	940.61	Joback Method
cpg	904.52	J/molxK	976.76	Joback Method
cpg	915.57	J/molxK	1012.91	Joback Method
cpg	925.46	J/molxK	1049.06	Joback Method
cpg	934.21	J/molxK	1085.21	Joback Method
cpg	941.84	J/molxK	1121.35	Joback Method
cpg	948.36	J/molxK	1157.50	Joback Method
dvisc	0.0002840	Paxs	601.95	Joback Method
dvisc	0.0001793	Paxs	658.39	Joback Method

dvisc	0.0001217	Paxs	714.84	Joback Method
dvisc	0.0000874	Paxs	771.28	Joback Method
dvisc	0.0000657	Paxs	827.72	Joback Method
dvisc	0.0000512	Paxs	884.17	Joback Method
dvisc	0.0000412	Paxs	940.61	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=U353911&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353911&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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