

# Adipic acid, 2-chloropropyl isoheptyl ester

**Inchi:** InChI=1S/C15H27ClO4/c1-12(2)7-6-10-19-14(17)8-4-5-9-15(18)20-11-13(3)16/h12-13H,  
**InchiKey:** ZMRLMLDKSVHUNW-UHFFFAOYSA-N  
**Formula:** C15H27ClO4  
**SMILES:** CC(C)CCCOC(=O)CCCCC(=O)OCC(C)Cl  
**Mol. weight [g/mol]:** 306.82

## Physical Properties

Property code	Value	Unit	Source
gf	-409.23	kJ/mol	Joback Method
hf	-868.83	kJ/mol	Joback Method
hfus	37.33	kJ/mol	Joback Method
hvap	70.91	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.697		Crippen Method
mvol	249.330	ml/mol	McGowan Method
pc	1494.19	kPa	Joback Method
rinpol	2019.00		NIST Webbook
tb	731.73	K	Joback Method
tc	916.63	K	Joback Method
tf	403.05	K	Joback Method
vc	0.961	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.21	J/molxK	731.73	Joback Method
cpg	724.89	J/molxK	762.55	Joback Method
cpg	739.70	J/molxK	793.36	Joback Method
cpg	753.67	J/molxK	824.18	Joback Method
cpg	766.81	J/molxK	855.00	Joback Method
cpg	779.11	J/molxK	885.81	Joback Method
cpg	790.58	J/molxK	916.63	Joback Method
dvisc	0.0016254	Paxs	403.05	Joback Method
dvisc	0.0007278	Paxs	457.83	Joback Method

dvisc	0.0003870	Paxs	512.61	Joback Method
dvisc	0.0002324	Paxs	567.39	Joback Method
dvisc	0.0001527	Paxs	622.17	Joback Method
dvisc	0.0001074	Paxs	676.95	Joback Method
dvisc	0.0000796	Paxs	731.73	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=U353541&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353541&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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