

# Adipic acid, butyl 2-chloropropyl ester

<b>Inchi:</b>	InChI=1S/C13H23ClO4/c1-3-4-9-17-12(15)7-5-6-8-13(16)18-10-11(2)14/h11H,3-10H2,1-
<b>InchiKey:</b>	GUVRUDLWCSXQOI-UHFFFAOYSA-N
<b>Formula:</b>	C13H23ClO4
<b>SMILES:</b>	CCCCOC(=O)CCCC(=O)OCC(C)Cl
<b>Mol. weight [g/mol]:</b>	278.77

## Physical Properties

Property code	Value	Unit	Source
gf	-423.63	kJ/mol	Joback Method
hf	-822.27	kJ/mol	Joback Method
hfus	35.67	kJ/mol	Joback Method
hvap	66.84	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.061		Crippen Method
mvol	221.150	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
rinpol	1848.00		NIST Webbook
rinpol	1848.00		NIST Webbook
tb	686.41	K	Joback Method
tc	869.92	K	Joback Method
tf	395.51	K	Joback Method
vc	0.855	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.84	J/mol×K	686.41	Joback Method
cpg	664.42	J/mol×K	839.33	Joback Method
cpg	652.76	J/mol×K	808.75	Joback Method
cpg	640.38	J/mol×K	778.16	Joback Method
cpg	627.27	J/mol×K	747.58	Joback Method
cpg	613.43	J/mol×K	716.99	Joback Method
cpg	675.35	J/mol×K	869.92	Joback Method
dvisc	0.0001131	Paxs	686.41	Joback Method

dvisc	0.0001488	Paxs	637.93	Joback Method
dvisc	0.0002049	Paxs	589.44	Joback Method
dvisc	0.0002988	Paxs	540.96	Joback Method
dvisc	0.0004693	Paxs	492.48	Joback Method
dvisc	0.0008133	Paxs	443.99	Joback Method
dvisc	0.0016130	Paxs	395.51	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=U353540&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353540&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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