

# Succinic acid, 4-chloro-2-nitrobenzyl hexyl ester

<b>Inchi:</b>	InChI=1S/C17H22ClNO6/c1-2-3-4-5-10-24-16(20)8-9-17(21)25-12-13-6-7-14(18)11-15(19)
<b>InchiKey:</b>	YOPFARBQHXDRJG-UHFFFAOYSA-N
<b>Formula:</b>	C17H22ClNO6
<b>SMILES:</b>	CCCCCCOC(=O)CCC(=O)OCc1ccc(Cl)cc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	371.81

## Physical Properties

Property code	Value	Unit	Source
gf	-258.81	kJ/mol	Joback Method
hf	-696.72	kJ/mol	Joback Method
hfus	54.18	kJ/mol	Joback Method
hvap	96.32	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	4.195		Crippen Method
mvol	271.170	ml/mol	McGowan Method
pc	1623.29	kPa	Joback Method
rinpol	2642.00		NIST Webbook
rinpol	2642.00		NIST Webbook
tb	966.85	K	Joback Method
tc	1194.49	K	Joback Method
tf	650.66	K	Joback Method
vc	1.058	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	831.77	J/mol×K	966.85	Joback Method
cpg	842.61	J/mol×K	1004.79	Joback Method
cpg	852.20	J/mol×K	1042.73	Joback Method
cpg	860.58	J/mol×K	1080.67	Joback Method
cpg	867.75	J/mol×K	1118.61	Joback Method
cpg	873.74	J/mol×K	1156.55	Joback Method
cpg	878.57	J/mol×K	1194.49	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=U380940&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380940&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>rinpola:</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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