

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

Inchi:	InChI=1S/C21H30ClNO6/c1-2-3-4-5-6-7-8-9-14-28-20(24)12-13-21(25)29-16-17-10-11-1
InchiKey:	RWZYGHOHFMZYMD-UHFFFAOYSA-N
Formula:	C21H30ClNO6
SMILES:	CCCCCCCCCOC(=O)CCC(=O)OCc1ccc(Cl)cc1[N+](=O)[O-]
Mol. weight [g/mol]:	427.92

## Physical Properties

Property code	Value	Unit	Source
gf	-225.13	kJ/mol	Joback Method
hf	-779.28	kJ/mol	Joback Method
hfus	64.54	kJ/mol	Joback Method
hvap	105.23	kJ/mol	Joback Method
log10ws	-7.27		Crippen Method
logp	5.755		Crippen Method
mcvol	327.530	ml/mol	McGowan Method
pc	1217.44	kPa	Joback Method
rinpol	3033.00		NIST Webbook
rinpol	3033.00		NIST Webbook
tb	1058.37	K	Joback Method
tc	1295.91	K	Joback Method
tf	695.74	K	Joback Method
vc	1.282	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1067.03	J/mol×K	1058.37	Joback Method
cpg	1078.26	J/mol×K	1097.96	Joback Method
cpg	1088.01	J/mol×K	1137.55	Joback Method
cpg	1096.30	J/mol×K	1177.14	Joback Method
cpg	1103.20	J/mol×K	1216.73	Joback Method
cpg	1108.74	J/mol×K	1256.32	Joback Method
cpg	1112.96	J/mol×K	1295.91	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=U380944&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380944&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>hvp:</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>rinp:</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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