

# Succinic acid, di(4-chloro-2-nitrobenzyl) ester

**Inchi:** InChI=1S/C18H14Cl2N2O8/c19-13-3-1-11(15(7-13)21(25)26)9-29-17(23)5-6-18(24)30-1  
**InchiKey:** POCUHZQODMUMII-UHFFFAOYSA-N  
**Formula:** C18H14Cl2N2O8  
**SMILES:** O=C(CCC(=O)OCc1ccc(Cl)cc1[N+](=O)[O-])OCc1ccc(Cl)cc1[N+](=O)[O-]  
**Mol. weight [g/mol]:** 457.22

## Physical Properties

Property code	Value	Unit	Source
gf	-133.62	kJ/mol	Joback Method
hf	-530.27	kJ/mol	Joback Method
hfus	65.59	kJ/mol	Joback Method
hvap	123.13	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	4.377		Crippen Method
mcvol	291.160	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
rinpol	3346.00		NIST Webbook
rinpol	3346.00		NIST Webbook
tb	1215.64	K	Joback Method
tc	1493.60	K	Joback Method
tf	886.92	K	Joback Method
vc	1.137	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.98	J/molxK	1215.64	Joback Method
cpg	853.46	J/molxK	1261.97	Joback Method
cpg	853.36	J/molxK	1308.29	Joback Method
cpg	851.73	J/molxK	1354.62	Joback Method
cpg	848.61	J/molxK	1400.94	Joback Method
cpg	844.07	J/molxK	1447.27	Joback Method
cpg	838.14	J/molxK	1493.60	Joback Method

# Sources

<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=U380946&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380946&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rin<sub>pol</sub>:</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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