

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

<b>Inchi:</b>	InChI=1S/C15H18ClNO6/c1-2-3-8-22-14(18)6-7-15(19)23-10-11-4-5-12(16)9-13(11)17(2)
<b>InchiKey:</b>	AVLFGZXCMKLHHJ-UHFFFAOYSA-N
<b>Formula:</b>	C15H18ClNO6
<b>SMILES:</b>	CCCCOC(=O)CCC(=O)OCc1ccc(Cl)cc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	343.76

## Physical Properties

Property code	Value	Unit	Source
gf	-275.65	kJ/mol	Joback Method
hf	-655.44	kJ/mol	Joback Method
hfus	49.00	kJ/mol	Joback Method
hvap	91.87	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	3.415		Crippen Method
mvol	242.990	ml/mol	McGowan Method
pc	1906.90	kPa	Joback Method
rinpol	2442.00		NIST Webbook
rinpol	2442.00		NIST Webbook
tb	921.09	K	Joback Method
tc	1149.20	K	Joback Method
tf	628.12	K	Joback Method
vc	0.947	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.52	J/molxK	921.09	Joback Method
cpg	728.07	J/molxK	959.11	Joback Method
cpg	737.46	J/molxK	997.13	Joback Method
cpg	745.71	J/molxK	1035.15	Joback Method
cpg	752.82	J/molxK	1073.16	Joback Method
cpg	758.81	J/molxK	1111.18	Joback Method
cpg	763.71	J/molxK	1149.20	Joback Method

# Sources

<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=U380937&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380937&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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