

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

<b>Inchi:</b>	InChI=1S/C15H18ClNO6/c1-10(2)8-22-14(18)5-6-15(19)23-9-11-3-4-12(16)7-13(11)17(2)
<b>InchiKey:</b>	DIMOVBVWYIYWOU-UHFFFAOYSA-N
<b>Formula:</b>	C15H18ClNO6
<b>SMILES:</b>	CC(C)COC(=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	-278.09	kJ/mol	Joback Method
hf	-660.72	kJ/mol	Joback Method
hfus	45.48	kJ/mol	Joback Method
hvap	91.48	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.271		Crippen Method
mvol	242.990	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	2395.00		NIST Webbook
rinpol	2395.00		NIST Webbook
tb	920.65	K	Joback Method
tc	1151.32	K	Joback Method
tf	613.12	K	Joback Method
vc	0.941	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	718.06	J/mol×K	920.65	Joback Method
cpg	728.68	J/mol×K	959.10	Joback Method
cpg	738.10	J/mol×K	997.54	Joback Method
cpg	746.34	J/mol×K	1035.99	Joback Method
cpg	753.40	J/mol×K	1074.43	Joback Method
cpg	759.31	J/mol×K	1112.88	Joback Method
cpg	764.08	J/mol×K	1151.32	Joback Method

# Sources

<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=U380936&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380936&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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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