

# Succinic acid, 3-methyl-4-nitrobenzyl propyl ester

<b>Inchi:</b>	InChI=1S/C15H19NO6/c1-3-8-21-14(17)6-7-15(18)22-10-12-4-5-13(16(19)20)11(2)9-12/
<b>InchiKey:</b>	LDIWEZXQECSDQW-UHFFFAOYSA-N
<b>Formula:</b>	C15H19NO6
<b>SMILES:</b>	CCCOC(=O)CCC(=O)OCc1ccc([N+](=O)[O-])c(C)c1
<b>Mol. weight [g/mol]:</b>	309.31

## Physical Properties

Property code	Value	Unit	Source
gf	-263.72	kJ/mol	Joback Method
hf	-639.70	kJ/mol	Joback Method
hfus	44.80	kJ/mol	Joback Method
hvap	87.49	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	2.680		Crippen Method
mvol	230.750	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	2349.00		NIST Webbook
rinpol	2349.00		NIST Webbook
tb	883.66	K	Joback Method
tc	1108.06	K	Joback Method
tf	598.20	K	Joback Method
vc	0.897	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.82	J/molxK	883.66	Joback Method
cpg	708.65	J/molxK	921.06	Joback Method
cpg	719.33	J/molxK	958.46	Joback Method
cpg	728.87	J/molxK	995.86	Joback Method
cpg	737.28	J/molxK	1033.26	Joback Method
cpg	744.57	J/molxK	1070.66	Joback Method
cpg	750.76	J/molxK	1108.06	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=U380978&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380978&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.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>

# 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>h vap:</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>r in pol:</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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