

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

<b>Inchi:</b>	InChI=1S/C14H17NO6/c1-3-20-13(16)6-7-14(17)21-9-11-5-4-10(2)12(8-11)15(18)19/h4-5
<b>InchiKey:</b>	RUKBUDXQQDIWMM-UHFFFAOYSA-N
<b>Formula:</b>	C14H17NO6
<b>SMILES:</b>	CCOC(=O)CCC(=O)OCc1ccc(C)c([N+](=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	295.29

## Physical Properties

Property code	Value	Unit	Source
gf	-272.14	kJ/mol	Joback Method
hf	-619.06	kJ/mol	Joback Method
hfus	42.21	kJ/mol	Joback Method
hvap	85.26	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	2.290		Crippen Method
mcvol	216.660	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
rinpol	2245.00		NIST Webbook
rinpol	2245.00		NIST Webbook
tb	860.78	K	Joback Method
tc	1087.02	K	Joback Method
tf	586.93	K	Joback Method
vc	0.842	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.86	J/molxK	860.78	Joback Method
cpg	652.48	J/molxK	898.49	Joback Method
cpg	662.99	J/molxK	936.19	Joback Method
cpg	672.40	J/molxK	973.90	Joback Method
cpg	680.70	J/molxK	1011.60	Joback Method
cpg	687.92	J/molxK	1049.31	Joback Method
cpg	694.05	J/molxK	1087.02	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.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>
<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=U381126&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381126&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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