

# Succinic acid, ethyl 3-nitrobenzyl ester

<b>Inchi:</b>	InChI=1S/C13H15NO6/c1-2-19-12(15)6-7-13(16)20-9-10-4-3-5-11(8-10)14(17)18/h3-5,8
<b>InchiKey:</b>	AJHATJNXYLTFX-UHFFFAOYSA-N
<b>Formula:</b>	C13H15NO6
<b>SMILES:</b>	CCOC(=O)CCC(=O)OCc1cccc([N+](=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	281.26

## Physical Properties

Property code	Value	Unit	Source
gf	-270.93	kJ/mol	Joback Method
hf	-586.95	kJ/mol	Joback Method
hfus	40.01	kJ/mol	Joback Method
hvap	82.37	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	1.981		Crippen Method
mcvol	202.570	ml/mol	McGowan Method
pc	2388.85	kPa	Joback Method
rinpol	2183.00		NIST Webbook
rinpol	2183.00		NIST Webbook
tb	832.92	K	Joback Method
tc	1060.93	K	Joback Method
tf	563.14	K	Joback Method
vc	0.785	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	587.32	J/mol×K	832.92	Joback Method
cpg	598.77	J/mol×K	870.92	Joback Method
cpg	609.15	J/mol×K	908.92	Joback Method
cpg	618.46	J/mol×K	946.92	Joback Method
cpg	626.72	J/mol×K	984.92	Joback Method
cpg	633.95	J/mol×K	1022.93	Joback Method
cpg	640.15	J/mol×K	1060.93	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=U381685&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381685&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>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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