

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

<b>Inchi:</b>	InChI=1S/C18H25NO6/c1-3-4-5-6-11-24-17(20)9-10-18(21)25-13-15-7-8-16(19(22)23)14
<b>InchiKey:</b>	VSIFPNTYHAVQCN-UHFFFAOYSA-N
<b>Formula:</b>	C18H25NO6
<b>SMILES:</b>	CCCCCOC(=O)CCC(=O)OCc1ccc([N+](=O)[O-])c(C)c1
<b>Mol. weight [g/mol]:</b>	351.39

## Physical Properties

Property code	Value	Unit	Source
gf	-238.46	kJ/mol	Joback Method
hf	-701.62	kJ/mol	Joback Method
hfus	52.57	kJ/mol	Joback Method
hvap	94.17	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	3.850		Crippen Method
mcvol	273.020	ml/mol	McGowan Method
pc	1548.78	kPa	Joback Method
rinpol	2643.00		NIST Webbook
rinpol	2643.00		NIST Webbook
tb	952.30	K	Joback Method
tc	1175.63	K	Joback Method
tf	632.01	K	Joback Method
vc	1.065	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	869.16	J/mol×K	952.30	Joback Method
cpg	881.41	J/mol×K	989.52	Joback Method
cpg	892.39	J/mol×K	1026.74	Joback Method
cpg	902.11	J/mol×K	1063.97	Joback Method
cpg	910.59	J/mol×K	1101.19	Joback Method
cpg	917.87	J/mol×K	1138.41	Joback Method
cpg	923.95	J/mol×K	1175.63	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=U380983&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380983&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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