

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

Inchi:	InChI=1S/C18H25NO7/c1-3-4-5-6-11-25-17(20)9-10-18(21)26-13-14-7-8-15(19(22)23)16
InchiKey:	INERTLNETKWWAT-UHFFFAOYSA-N
Formula:	C18H25NO7
SMILES:	CCCCCOC(=O)CCC(=O)OCc1ccc([N+](=O)[O-])c(OC)c1
Mol. weight [g/mol]:	367.39

## Physical Properties

Property code	Value	Unit	Source
gf	-343.46	kJ/mol	Joback Method
hf	-833.84	kJ/mol	Joback Method
hfus	53.76	kJ/mol	Joback Method
hvap	96.58	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	3.550		Crippen Method
mcvol	278.890	ml/mol	McGowan Method
pc	1528.27	kPa	Joback Method
rinsol	2797.00		NIST Webbook
rinsol	2797.00		NIST Webbook
tb	974.72	K	Joback Method
tc	1199.63	K	Joback Method
tf	654.24	K	Joback Method
vc	1.083	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	895.30	J/molxK	974.72	Joback Method
cpg	906.67	J/molxK	1012.21	Joback Method
cpg	916.61	J/molxK	1049.69	Joback Method
cpg	925.11	J/molxK	1087.18	Joback Method
cpg	932.18	J/molxK	1124.66	Joback Method
cpg	937.84	J/molxK	1162.15	Joback Method
cpg	942.07	J/molxK	1199.63	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=U381015&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381015&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>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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