

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

<b>Inchi:</b>	InChI=1S/C17H23NO7/c1-3-4-5-10-24-16(19)8-9-17(20)25-12-13-6-7-14(18(21)22)15(11)
<b>InchiKey:</b>	YDMCDPRWIKAGGD-UHFFFAOYSA-N
<b>Formula:</b>	C17H23NO7
<b>SMILES:</b>	CCCCCOC(=O)CCC(=O)OCc1ccc([N+](=O)[O-])c(OC)c1
<b>Mol. weight [g/mol]:</b>	353.37

## Physical Properties

Property code	Value	Unit	Source
gf	-351.88	kJ/mol	Joback Method
hf	-813.20	kJ/mol	Joback Method
hfus	51.17	kJ/mol	Joback Method
hvap	94.35	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	3.160		Crippen Method
mvol	264.800	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
rinpol	2697.00		NIST Webbook
rinpol	2697.00		NIST Webbook
tb	951.84	K	Joback Method
tc	1175.57	K	Joback Method
tf	642.97	K	Joback Method
vc	1.028	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	837.16	J/molxK	951.84	Joback Method
cpg	848.49	J/molxK	989.13	Joback Method
cpg	858.45	J/molxK	1026.42	Joback Method
cpg	867.04	J/molxK	1063.71	Joback Method
cpg	874.26	J/molxK	1100.99	Joback Method
cpg	880.11	J/molxK	1138.28	Joback Method
cpg	884.59	J/molxK	1175.57	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=U381013&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381013&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>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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