

# Succinic acid, 3-methoxy-4-nitrobenzyl 2-methylhex-3-yl ester

<b>Inchi:</b>	InChI=1S/C19H27NO7/c1-5-6-16(13(2)3)27-19(22)10-9-18(21)26-12-14-7-8-15(20(23)24
<b>InchiKey:</b>	SQDBYVSJCFEROY-UHFFFAOYSA-N
<b>Formula:</b>	C19H27NO7
<b>SMILES:</b>	CCCC(OC(=O)CCC(=O)OCc1ccc([N+](=O)[O-])c(OC)c1)C(C)C
<b>Mol. weight [g/mol]:</b>	381.42

## Physical Properties

Property code	Value	Unit	Source
gf	-339.92	kJ/mol	Joback Method
hf	-865.04	kJ/mol	Joback Method
hfus	49.31	kJ/mol	Joback Method
hvap	98.02	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	3.795		Crippen Method
mcvol	292.980	ml/mol	McGowan Method
pc	1436.98	kPa	Joback Method
rinpol	2753.00		NIST Webbook
rinpol	2753.00		NIST Webbook
tb	996.72	K	Joback Method
tc	1225.89	K	Joback Method
tf	635.51	K	Joback Method
vc	1.127	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	954.76	J/molxK	996.72	Joback Method
cpg	966.12	J/molxK	1034.91	Joback Method
cpg	975.92	J/molxK	1073.11	Joback Method
cpg	984.16	J/molxK	1111.30	Joback Method
cpg	990.84	J/molxK	1149.50	Joback Method
cpg	995.99	J/molxK	1187.69	Joback Method
cpg	999.60	J/molxK	1225.89	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=U381014&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381014&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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