

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

<b>Inchi:</b>	InChI=1S/C18H25NO6/c1-4-5-16(13(2)3)25-18(21)11-10-17(20)24-12-14-6-8-15(9-7-14)
<b>InchiKey:</b>	GQODUCLWMWAXMQ-UHFFFAOYSA-N
<b>Formula:</b>	C18H25NO6
<b>SMILES:</b>	CCCC(OC(=O)CCC(=O)OCc1ccc([N+](=O)[O-])cc1)C(C)C
<b>Mol. weight [g/mol]:</b>	351.39

## Physical Properties

Property code	Value	Unit	Source
gf	-233.71	kJ/mol	Joback Method
hf	-700.71	kJ/mol	Joback Method
hfus	45.92	kJ/mol	Joback Method
hvap	92.73	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	3.786		Crippen Method
mvol	273.020	ml/mol	McGowan Method
pc	1587.28	kPa	Joback Method
rinpol	2557.00		NIST Webbook
rinpol	2557.00		NIST Webbook
tb	946.44	K	Joback Method
tc	1172.55	K	Joback Method
tf	589.49	K	Joback Method
vc	1.054	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.42	J/molxK	946.44	Joback Method
cpg	883.89	J/molxK	984.13	Joback Method
cpg	895.04	J/molxK	1021.81	Joback Method
cpg	904.89	J/molxK	1059.50	Joback Method
cpg	913.48	J/molxK	1097.18	Joback Method
cpg	920.85	J/molxK	1134.87	Joback Method
cpg	927.01	J/molxK	1172.55	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U381170&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381170&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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