

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

<b>Inchi:</b>	InChI=1S/C19H27NO6/c1-5-6-17(13(2)3)26-19(22)10-9-18(21)25-12-15-8-7-14(4)16(11-
<b>InchiKey:</b>	GAJAFEPTQNTALM-UHFFFAOYSA-N
<b>Formula:</b>	C19H27NO6
<b>SMILES:</b>	CCCC(OC(=O)CCC(=O)OCc1ccc(C)c([N+](=O)[O-])c1)C(C)C
<b>Mol. weight [g/mol]:</b>	365.42

## Physical Properties

Property code	Value	Unit	Source
gf	-234.92	kJ/mol	Joback Method
hf	-732.82	kJ/mol	Joback Method
hfus	48.12	kJ/mol	Joback Method
hvap	95.61	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	4.095		Crippen Method
mcvol	287.110	ml/mol	McGowan Method
pc	1455.68	kPa	Joback Method
rinpol	2588.00		NIST Webbook
rinpol	2588.00		NIST Webbook
tb	974.30	K	Joback Method
tc	1201.77	K	Joback Method
tf	613.28	K	Joback Method
vc	1.109	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	928.74	J/molxK	974.30	Joback Method
cpg	941.13	J/molxK	1012.21	Joback Method
cpg	952.13	J/molxK	1050.12	Joback Method
cpg	961.77	J/molxK	1088.03	Joback Method
cpg	970.07	J/molxK	1125.95	Joback Method
cpg	977.05	J/molxK	1163.86	Joback Method
cpg	982.75	J/molxK	1201.77	Joback Method

# Sources

<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=U381131&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381131&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>

# 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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