

# Succinic acid, butyl 3-methyl-4-nitrobenzyl ester

<b>Inchi:</b>	InChI=1S/C16H21NO6/c1-3-4-9-22-15(18)7-8-16(19)23-11-13-5-6-14(17(20)21)12(2)10-
<b>InchiKey:</b>	FLYDIYGKHHGSDBK-UHFFFAOYSA-N
<b>Formula:</b>	C16H21NO6
<b>SMILES:</b>	CCCCOC(=O)CCC(=O)OCc1ccc([N+](=O)[O-])c(C)c1
<b>Mol. weight [g/mol]:</b>	323.34

## Physical Properties

Property code	Value	Unit	Source
gf	-255.30	kJ/mol	Joback Method
hf	-660.34	kJ/mol	Joback Method
hfus	47.39	kJ/mol	Joback Method
hvap	89.71	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.070		Crippen Method
mvol	244.840	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
rinpol	2447.00		NIST Webbook
rinpol	2447.00		NIST Webbook
tb	906.54	K	Joback Method
tc	1129.81	K	Joback Method
tf	609.47	K	Joback Method
vc	0.954	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.56	J/mol×K	906.54	Joback Method
cpg	765.56	J/mol×K	943.75	Joback Method
cpg	776.37	J/mol×K	980.96	Joback Method
cpg	786.01	J/mol×K	1018.18	Joback Method
cpg	794.48	J/mol×K	1055.39	Joback Method
cpg	801.81	J/mol×K	1092.60	Joback Method
cpg	808.00	J/mol×K	1129.81	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U380980&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380980&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>hvpap:</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>rinppl:</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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