

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

<b>Inchi:</b>	InChI=1S/C16H21NO7/c1-3-4-9-23-15(18)7-8-16(19)24-11-12-5-6-14(22-2)13(10-12)17(
<b>InchiKey:</b>	VMJMDLYUJGLDEJ-UHFFFAOYSA-N
<b>Formula:</b>	C16H21NO7
<b>SMILES:</b>	CCCCOC(=O)CCC(=O)OCc1ccc(OC)c([N+](=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	339.34

## Physical Properties

Property code	Value	Unit	Source
gf	-360.30	kJ/mol	Joback Method
hf	-792.56	kJ/mol	Joback Method
hfus	48.58	kJ/mol	Joback Method
hvap	92.12	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	2.770		Crippen Method
mcvol	250.710	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
rinpol	2624.00		NIST Webbook
rinpol	2624.00		NIST Webbook
tb	928.96	K	Joback Method
tc	1152.36	K	Joback Method
tf	631.70	K	Joback Method
vc	0.972	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.58	J/mol×K	928.96	Joback Method
cpg	790.85	J/mol×K	966.19	Joback Method
cpg	800.81	J/mol×K	1003.43	Joback Method
cpg	809.44	J/mol×K	1040.66	Joback Method
cpg	816.76	J/mol×K	1077.89	Joback Method
cpg	822.76	J/mol×K	1115.13	Joback Method
cpg	827.43	J/mol×K	1152.36	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U380949&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380949&amp;Units=SI</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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