

# Succinic acid, 2-nitrobenzyl pentyl ester

<b>Inchi:</b>	InChI=1S/C16H21NO6/c1-2-3-6-11-22-15(18)9-10-16(19)23-12-13-7-4-5-8-14(13)17(20)
<b>InchiKey:</b>	PLSYBHGYRNGTTG-UHFFFAOYSA-N
<b>Formula:</b>	C16H21NO6
<b>SMILES:</b>	CCCCCOC(=O)CCC(=O)OCc1ccccc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	323.34

## Physical Properties

Property code	Value	Unit	Source
gf	-245.67	kJ/mol	Joback Method
hf	-648.87	kJ/mol	Joback Method
hfus	47.78	kJ/mol	Joback Method
hvap	89.05	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.152		Crippen Method
mvol	244.840	ml/mol	McGowan Method
pc	1835.69	kPa	Joback Method
rmpol	2429.00		NIST Webbook
rmpol	2429.00		NIST Webbook
tb	901.56	K	Joback Method
tc	1124.04	K	Joback Method
tf	596.95	K	Joback Method
vc	0.954	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	754.95	J/molxK	901.56	Joback Method
cpg	767.04	J/molxK	938.64	Joback Method
cpg	777.96	J/molxK	975.72	Joback Method
cpg	787.73	J/molxK	1012.80	Joback Method
cpg	796.37	J/molxK	1049.88	Joback Method
cpg	803.89	J/molxK	1086.96	Joback Method
cpg	810.33	J/molxK	1124.04	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=U380897&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380897&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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