

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

<b>Inchi:</b>	InChI=1S/C22H33NO6/c1-3-4-5-6-7-8-9-10-15-28-21(24)13-14-22(25)29-17-19-11-12-20
<b>InchiKey:</b>	FWUNUEZQNFGLC-UHFFFAOYSA-N
<b>Formula:</b>	C22H33NO6
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCC(=O)OCc1ccc([N+](=O)[O-])c(C)c1
<b>Mol. weight [g/mol]:</b>	407.50

## Physical Properties

Property code	Value	Unit	Source
gf	-204.78	kJ/mol	Joback Method
hf	-784.18	kJ/mol	Joback Method
hfus	62.93	kJ/mol	Joback Method
hvap	103.07	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	5.411		Crippen Method
mcvol	329.380	ml/mol	McGowan Method
pc	1168.82	kPa	Joback Method
rinpol	3040.00		NIST Webbook
rinpol	3040.00		NIST Webbook
tb	1043.82	K	Joback Method
tc	1278.00	K	Joback Method
tf	677.09	K	Joback Method
vc	1.290	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1107.06	J/molxK	1043.82	Joback Method
cpg	1119.70	J/molxK	1082.85	Joback Method
cpg	1130.80	J/molxK	1121.88	Joback Method
cpg	1140.40	J/molxK	1160.91	Joback Method
cpg	1148.56	J/molxK	1199.94	Joback Method
cpg	1155.30	J/molxK	1238.97	Joback Method
cpg	1160.68	J/molxK	1278.00	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=U380987&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380987&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>hvap:</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>rinpola:</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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