

# Succinic acid, 3-methylbut-2-yl 3-nitrobenzyl ester

<b>Inchi:</b>	InChI=1S/C16H21NO6/c1-11(2)12(3)23-16(19)8-7-15(18)22-10-13-5-4-6-14(9-13)17(20)
<b>InchiKey:</b>	RDGDBSPRCWADRH-UHFFFAOYSA-N
<b>Formula:</b>	C16H21NO6
<b>SMILES:</b>	CC(C)C(C)OC(=O)CCC(=O)OCc1cccc([N+](=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	323.34

## Physical Properties

Property code	Value	Unit	Source
gf	-250.55	kJ/mol	Joback Method
hf	-659.43	kJ/mol	Joback Method
hfus	40.74	kJ/mol	Joback Method
hvap	88.27	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.006		Crippen Method
mcvol	244.840	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpola	2431.00		NIST Webbook
rinpola	2431.00		NIST Webbook
tb	900.68	K	Joback Method
tc	1128.23	K	Joback Method
tf	566.95	K	Joback Method
vc	0.942	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.02	J/molxK	900.68	Joback Method
cpg	768.32	J/molxK	938.61	Joback Method
cpg	779.35	J/molxK	976.53	Joback Method
cpg	789.16	J/molxK	1014.46	Joback Method
cpg	797.75	J/molxK	1052.38	Joback Method
cpg	805.16	J/molxK	1090.31	Joback Method
cpg	811.41	J/molxK	1128.23	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=U390178&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390178&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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