

# Succinic acid, isobutyl 2-nitrobenzyl ester

**Inchi:** InChI=1S/C15H19NO6/c1-11(2)9-21-14(17)7-8-15(18)22-10-12-5-3-4-6-13(12)16(19)20/  
**InchiKey:** YVEKQJGVCCNOCB-UHFFFAOYSA-N  
**Formula:** C15H19NO6  
**SMILES:** CC(C)COC(=O)CCC(=O)OCc1ccccc1[N+](=O)[O-]  
**Mol. weight [g/mol]:** 309.31

## Physical Properties

Property code	Value	Unit	Source
gf	-256.53	kJ/mol	Joback Method
hf	-633.51	kJ/mol	Joback Method
hfus	41.67	kJ/mol	Joback Method
hvap	86.44	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	2.617		Crippen Method
mcvol	230.750	ml/mol	McGowan Method
pc	2010.90	kPa	Joback Method
rinpol	2286.00		NIST Webbook
rinpol	2286.00		NIST Webbook
tb	878.24	K	Joback Method
tc	1104.68	K	Joback Method
tf	570.68	K	Joback Method
vc	0.891	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.81	J/mol×K	878.24	Joback Method
cpg	710.85	J/mol×K	915.98	Joback Method
cpg	721.71	J/mol×K	953.72	Joback Method
cpg	731.40	J/mol×K	991.46	Joback Method
cpg	739.95	J/mol×K	1029.20	Joback Method
cpg	747.37	J/mol×K	1066.94	Joback Method
cpg	753.69	J/mol×K	1104.68	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U380895&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380895&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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