

# Succinic acid, heptyl 2-nitrobenzyl ester

<b>Inchi:</b>	InChI=1S/C18H25NO6/c1-2-3-4-5-8-13-24-17(20)11-12-18(21)25-14-15-9-6-7-10-16(15)
<b>InchiKey:</b>	MJIUKBPVWIARNJ-UHFFFAOYSA-N
<b>Formula:</b>	C18H25NO6
<b>SMILES:</b>	CCCCCCCOC(=O)CCC(=O)OCc1ccccc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	351.39

## Physical Properties

Property code	Value	Unit	Source
gf	-228.83	kJ/mol	Joback Method
hf	-690.15	kJ/mol	Joback Method
hfus	52.96	kJ/mol	Joback Method
hvap	93.50	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	3.932		Crippen Method
mvol	273.020	ml/mol	McGowan Method
pc	1567.23	kPa	Joback Method
rinpol	2633.00		NIST Webbook
rinpol	2633.00		NIST Webbook
tb	947.32	K	Joback Method
tc	1169.79	K	Joback Method
tf	619.49	K	Joback Method
vc	1.065	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.47	J/mol×K	947.32	Joback Method
cpg	882.84	J/mol×K	984.40	Joback Method
cpg	893.96	J/mol×K	1021.48	Joback Method
cpg	903.85	J/mol×K	1058.56	Joback Method
cpg	912.55	J/mol×K	1095.64	Joback Method
cpg	920.08	J/mol×K	1132.72	Joback Method
cpg	926.47	J/mol×K	1169.79	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U380900&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380900&amp;Units=SI</a>
<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.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>

# 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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