

# Succinic acid, hex-4-yn-3-yl 3-nitrophenyl ester

Inchi:	InChI=1S/C16H17NO6/c1-3-6-13(4-2)22-15(18)9-10-16(19)23-14-8-5-7-12(11-14)17(20)
InchiKey:	BDCGPQGBSSSLQB-UHFFFAOYSA-N
Formula:	C16H17NO6
SMILES:	CC#CC(CC)OC(=O)CCC(=O)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	319.31

## Physical Properties

Property code	Value	Unit	Source
gf	-45.31	kJ/mol	Joback Method
hf	-381.85	kJ/mol	Joback Method
hfus	47.38	kJ/mol	Joback Method
hvap	90.81	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	2.625		Crippen Method
mcvol	236.240	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	2474.00		NIST Webbook
rinpol	2474.00		NIST Webbook
tb	910.12	K	Joback Method
tc	1151.47	K	Joback Method
tf	688.05	K	Joback Method
vc	0.909	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.22	J/molxK	910.12	Joback Method
cpg	711.61	J/molxK	950.34	Joback Method
cpg	721.72	J/molxK	990.57	Joback Method
cpg	730.56	J/molxK	1030.79	Joback Method
cpg	738.15	J/molxK	1071.02	Joback Method
cpg	744.52	J/molxK	1111.24	Joback Method
cpg	749.68	J/molxK	1151.47	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=U390136&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390136&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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