

# Benzeneacetic acid, 4-nitro-, 2,7-dimethyloct-1-en-3-yn-5-yl ester

**Inchi:** InChI=1S/C18H21NO4/c1-13(2)5-10-17(11-14(3)4)23-18(20)12-15-6-8-16(9-7-15)19(21)

**InchiKey:** WSVRONZAOIKFHC-UHFFFAOYSA-N

**Formula:** C18H21NO4

**SMILES:** C=C(C)C#CC(CC(C)C)OC(=O)Cc1ccc([N+](=O)[O-])cc1

**Mol. weight [g/mol]:** 315.36

## Physical Properties

Property code	Value	Unit	Source
gf	282.30	kJ/mol	Joback Method
hf	-67.97	kJ/mol	Joback Method
hfus	43.66	kJ/mol	Joback Method
hvap	85.13	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	3.675		Crippen Method
mcvol	252.680	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
rinsol	2284.00		NIST Webbook
tb	875.71	K	Joback Method
tc	1117.79	K	Joback Method
tf	607.71	K	Joback Method
vc	0.974	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.97	J/mol×K	875.71	Joback Method
cpg	765.32	J/mol×K	916.06	Joback Method
cpg	778.45	J/mol×K	956.40	Joback Method
cpg	790.41	J/mol×K	996.75	Joback Method
cpg	801.26	J/mol×K	1037.10	Joback Method
cpg	811.08	J/mol×K	1077.45	Joback Method
cpg	819.91	J/mol×K	1117.79	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=U406980&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406980&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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