

# Heptyl 4-nitrophenyl ether

<b>Other names:</b>	p-Heptyloxynitrobenzene p-n-Heptyloxynitrobenzene Benzene, 1-(heptyloxy)-4-nitro- p-Nitrophenyl heptyl ether
<b>Inchi:</b>	InChI=1S/C13H19NO3/c1-2-3-4-5-6-11-17-13-9-7-12(8-10-13)14(15)16/h7-10H,2-6,11H2
<b>InchiKey:</b>	AVDKYVSWJDZALX-UHFFFAOYSA-N
<b>Formula:</b>	C13H19NO3
<b>SMILES:</b>	CCCCCCCOc1ccc([N+](=O)[O-])cc1
<b>Mol. weight [g/mol]:</b>	237.29
<b>CAS:</b>	13565-36-1

## Physical Properties

Property code	Value	Unit	Source
gf	91.91	kJ/mol	Joback Method
hf	-229.57	kJ/mol	Joback Method
hfus	35.63	kJ/mol	Joback Method
hvap	66.47	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	3.944		Crippen Method
mcvol	193.560	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
tb	702.76	K	Joback Method
tc	921.69	K	Joback Method
tf	441.05	K	Joback Method
vc	0.755	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.35	J/molxK	702.76	Joback Method
cpg	550.68	J/molxK	739.25	Joback Method
cpg	565.01	J/molxK	775.74	Joback Method
cpg	578.38	J/molxK	812.22	Joback Method
cpg	590.82	J/molxK	848.71	Joback Method

cpg	602.36	J/mol×K	885.20	Joback Method
cpg	613.04	J/mol×K	921.69	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	438.50 ± 0.50	K	0.07	NIST Webbook

## 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=C13565361&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13565361&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>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>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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