

# p-Octyloxynitrobenzene

<b>Other names:</b>	p-Nitrophenyl octyl ether
<b>Inchi:</b>	InChI=1S/C14H21NO3/c1-2-3-4-5-6-7-12-18-14-10-8-13(9-11-14)15(16)17/h8-11H,2-7,1
<b>InchiKey:</b>	WTTNDGCMXADGCJ-UHFFFAOYSA-N
<b>Formula:</b>	C14H21NO3
<b>SMILES:</b>	CCCCCCCCOc1ccc([N+](=O)[O-])cc1
<b>Mol. weight [g/mol]:</b>	251.32
<b>CAS:</b>	49562-76-7

## Physical Properties

Property code	Value	Unit	Source
gf	100.33	kJ/mol	Joback Method
hf	-250.21	kJ/mol	Joback Method
hfus	38.22	kJ/mol	Joback Method
hvap	68.70	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.334		Crippen Method
mcvol	207.650	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
tb	725.64	K	Joback Method
tc	941.26	K	Joback Method
tf	452.32	K	Joback Method
vc	0.811	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.01	J/mol×K	725.64	Joback Method
cpg	604.71	J/mol×K	761.58	Joback Method
cpg	619.39	J/mol×K	797.51	Joback Method
cpg	633.10	J/mol×K	833.45	Joback Method
cpg	645.85	J/mol×K	869.39	Joback Method
cpg	657.69	J/mol×K	905.32	Joback Method
cpg	668.66	J/mol×K	941.26	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	496.00 ± 1.00	K	2.00	NIST Webbook

## Sources

<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=C49562767&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C49562767&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>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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