

# Butyl 4-nitrophenyl ether

<b>Other names:</b>	p-Nitrophenyl butyl ether n-Butyl 4-nitrophenyl ether p-Butoxynitrobenzene 4-n-Butoxynitrobenzene
<b>Inchi:</b>	InChI=1S/C10H13NO3/c1-2-3-8-14-10-6-4-9(5-7-10)11(12)13/h4-7H,2-3,8H2,1H3
<b>InchiKey:</b>	XCCDVZINDJESR-UHFFFAOYSA-N
<b>Formula:</b>	C10H13NO3
<b>SMILES:</b>	CCCCOc1ccc([N+](=O)[O-])cc1
<b>Mol. weight [g/mol]:</b>	195.22
<b>CAS:</b>	7244-78-2

## Physical Properties

Property code	Value	Unit	Source
gf	66.65	kJ/mol	Joback Method
hf	-167.65	kJ/mol	Joback Method
hfus	27.86	kJ/mol	Joback Method
hvap	59.79	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	2.774		Crippen Method
mcvol	151.290	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
tb	634.12	K	Joback Method
tc	865.31	K	Joback Method
tf	407.24	K	Joback Method
vc	0.588	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.25	J/molxK	634.12	Joback Method
cpg	395.94	J/molxK	672.65	Joback Method
cpg	408.72	J/molxK	711.18	Joback Method
cpg	420.63	J/molxK	749.72	Joback Method
cpg	431.69	J/molxK	788.25	Joback Method

cpg	441.93	J/mol×K	826.78	Joback Method
cpg	451.36	J/mol×K	865.31	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	447.50 ± 0.50	K	2.00	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=C7244782&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7244782&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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