

# Benzene, 1-(dimethoxymethyl)-2-nitro-

<b>Inchi:</b>	InChI=1S/C9H11NO4/c1-13-9(14-2)7-5-3-4-6-8(7)10(11)12/h3-6,9H,1-2H3
<b>InchiKey:</b>	OAPZTGKQZKPVPF-UHFFFAOYSA-N
<b>Formula:</b>	C9H11NO4
<b>SMILES:</b>	COC(OC)c1ccccc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	197.19
<b>CAS:</b>	20627-73-0

## Physical Properties

Property code	Value	Unit	Source
gf	-49.21	kJ/mol	Joback Method
hf	-284.51	kJ/mol	Joback Method
hfus	22.93	kJ/mol	Joback Method
hvap	59.59	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	1.886		Crippen Method
mcvol	143.070	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
tb	548.20	K	NIST Webbook
tc	870.66	K	Joback Method
tf	403.20	K	Joback Method
vc	0.543	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.19	J/molxK	633.22	Joback Method
cpg	371.21	J/molxK	672.79	Joback Method
cpg	383.37	J/molxK	712.37	Joback Method
cpg	394.66	J/molxK	751.94	Joback Method
cpg	405.08	J/molxK	791.51	Joback Method
cpg	414.65	J/molxK	831.09	Joback Method
cpg	423.35	J/molxK	870.66	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	411.70	K	1.50	NIST Webbook

## Sources

Joback Method:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C20627730&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C20627730&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<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>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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