

# 1-Nitro-2-propylbenzene

<b>Other names:</b>	Benzene, 1-nitro-2-propyl- o-Propylnitrobenzene o-Nitropropylbenzene
<b>Inchi:</b>	InChI=1S/C9H11NO2/c1-2-5-8-6-3-4-7-9(8)10(11)12/h3-4,6-7H,2,5H2,1H3
<b>InchiKey:</b>	UGAXDAGIKIVCQB-UHFFFAOYSA-N
<b>Formula:</b>	C9H11NO2
<b>SMILES:</b>	CCc1ccccc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	165.19
<b>CAS:</b>	7137-54-4

## Physical Properties

Property code	Value	Unit	Source
gf	163.23	kJ/mol	Joback Method
hf	-14.79	kJ/mol	Joback Method
hfus	24.08	kJ/mol	Joback Method
hvap	55.16	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.547		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3250.43	kPa	Joback Method
ripol	1969.00		NIST Webbook
tb	588.82	K	Joback Method
tc	828.33	K	Joback Method
tf	373.74	K	Joback Method
vc	0.513	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.78	J/molxK	588.82	Joback Method
cpg	323.96	J/molxK	628.74	Joback Method
cpg	336.22	J/molxK	668.66	Joback Method
cpg	347.61	J/molxK	708.57	Joback Method
cpg	358.16	J/molxK	748.49	Joback Method

cpg	367.92	J/mol×K	788.41	Joback Method
cpg	376.94	J/mol×K	828.33	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	407.70	K	3.50	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=C7137544&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7137544&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>
<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>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>ripol:</b>	Polar retention indices
<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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