

# 1-tert-Butyl-2-nitrobenzene

<b>Other names:</b>	Benzene, 1-(1,1-dimethylethyl)-2-nitro-1-tert-Butyl-4-nitrobenzene
<b>Inchi:</b>	InChI=1S/C10H13NO2/c1-10(2,3)8-6-4-5-7-9(8)11(12)13/h4-7H,1-3H3
<b>InchiKey:</b>	IWTHGPTVKBEURV-UHFFFAOYSA-N
<b>Formula:</b>	C10H13NO2
<b>SMILES:</b>	CC(C)(C)c1ccccc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	179.22
<b>CAS:</b>	1886-57-3

## Physical Properties

Property code	Value	Unit	Source
gf	174.49	kJ/mol	Joback Method
hf	-44.18	kJ/mol	Joback Method
hfus	19.26	kJ/mol	Joback Method
hvap	65.00 ± 0.60	kJ/mol	NIST Webbook
log10ws	-3.44		Crippen Method
logp	2.892		Crippen Method
mvol	145.420	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
tb	608.47	K	Joback Method
tc	858.26	K	Joback Method
tf	387.43	K	Joback Method
vc	0.558	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.51	J/mol×K	608.47	Joback Method
cpg	376.25	J/mol×K	650.10	Joback Method
cpg	389.79	J/mol×K	691.73	Joback Method
cpg	402.22	J/mol×K	733.36	Joback Method
cpg	413.64	J/mol×K	775.00	Joback Method
cpg	424.12	J/mol×K	816.63	Joback Method
cpg	433.75	J/mol×K	858.26	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	523.70	K	102.00	NIST Webbook
tbrp	387.70	K	1.30	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=C1886573&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1886573&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>hvapt:</b>	Enthalpy of vaporization at a given temperature
<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

<https://www.cheméo.com/cid/63-274-8/1-tert-Butyl-2-nitrobenzene.pdf>

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