Benzene, 1-(1-methylethyl)-4-nitro-

Other names:	1-(1-Methylethyl)-4-nitrobenzene
	1-Isopropyl-4-nitrobenzene
	2-(p-Nitrophenyl)propane
	4-Isopropylnitrobenzene
	4-Nitrocumene
	4-Nitroisopropylbenzene
	Cumene, p-nitro-
	NSC 14494
	p-Isopropylnitrobenzene
	p-Nitrocumene
	p-Nitroisopropylbenzene
Inchi:	InChI=1S/C9H11NO2/c1-7(2)8-3-5-9(6-4-8)10(11)12/h3-7H,1-2H3
InchiKey:	JXMYUMNAEKRMIP-UHFFFAOYSA-N
Formula:	C9H11NO2
SMILES:	CC(C)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	165.19
CAS:	1817-47-6

Physical Properties

Property code	Value	Unit	Source
gf	160.79	kJ/mol	Joback Method
hf	-20.07	kJ/mol	Joback Method
hfus	20.56	kJ/mol	Joback Method
hvap	54.77	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.718		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
tb	588.38	K	Joback Method
tc	833.34	K	Joback Method
tf	358.74	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.23	J/mol×K	588.38	Joback Method
cpg	324.77	J/mol×K	629.21	Joback Method
cpg	337.33	J/mol×K	670.03	Joback Method
cpg	348.96	J/mol×K	710.86	Joback Method
cpg	359.71	J/mol×K	751.69	Joback Method
cpg	369.63	J/mol×K	792.51	Joback Method
cpg	378.76	J/mol×K	833.34	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	379.70	K	1.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43515e+01
Coeff. B	-4.36379e+03
Coeff. C	-8.78370e+01
Temperature range (K), min.	398.12
Temperature range (K), max.	570.56

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1817476&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume