Benzene, 1-methoxy-3-nitro-

Other names:	Anisole, m-nitro-
	m-Methoxynitrobenzene
	m-Nitroanisole
	1-Methoxy-3-nitrobenzene
	3-Methoxynitrobenzene
	3-Nitroanisole
	Methyl m-nitrophenyl ether
	NSC 4956
Inchi:	InChI=1S/C7H7NO3/c1-11-7-4-2-3-6(5-7)8(9)10/h2-5H,1H3
InchiKey:	WGYFINWERLNPHR-UHFFFAOYSA-N
Formula:	C7H7NO3
SMILES:	COc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	153.14
CAS:	555-03-3

Physical Properties

Property code	Value	Unit	Source
ea	1.04 ± 0.10	eV	NIST Webbook
gf	41.39	kJ/mol	Joback Method
hf	-105.73	kJ/mol	Joback Method
hfus	20.09	kJ/mol	Joback Method
hvap	53.12	kJ/mol	Joback Method
ie	9.10 ± 0.10	eV	NIST Webbook
ie	9.01	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
log10ws	-2.24		Crippen Method
logp	1.603		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
pc	4010.84	kPa	Joback Method
rinpol	228.00		NIST Webbook
rinpol	1346.10		NIST Webbook
rinpol	228.00		NIST Webbook
rinpol	1346.10		NIST Webbook
rinpol	1273.00		NIST Webbook
tb	531.20	K	NIST Webbook
tc	811.60	K	Joback Method
tf	311.15 ± 1.50	K	NIST Webbook

vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.84	J/mol×K	565.48	Joback Method
cpg	253.81	J/mol×K	606.50	Joback Method
cpg	264.03	J/mol×K	647.52	Joback Method
cpg	273.53	J/mol×K	688.54	Joback Method
cpg	282.32	J/mol×K	729.56	Joback Method
cpg	290.41	J/mol×K	770.58	Joback Method
cpg	297.83	J/mol×K	811.60	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	395.20	K	1.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C555033&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
ea: Electron affinity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume