Benzene, 1-methoxy-4-nitro-

Other names:	1-Methoxy-4-nitrobenzene
	4-Methoxy-1-nitrobenzene
	4-Methoxynitrobenzene
	4-Nitro-1-methoxybenzene
	4-Nitroanisole
	4-Nitrophenyl methyl ether
	721942-42-3
	Anisole, p-nitro-
	Methyl 4-nitrophenyl ether
	Methyl p-nitrophenyl ether
	NSC 5507
	Nitroanisole
	Phenol, 4-nitro-, methylated
	UN 2730
	anisole, 4-nitro-
	p-Methoxynitrobenzene
	p-Nitroanisol
	p-Nitroanisole
	p-Nitromethoxybenzene
Inchi:	InChI=1S/C7H7NO3/c1-11-7-4-2-6(3-5-7)8(9)10/h2-5H,1H3
InchiKey:	BNUHAJGCKIQFGE-UHFFFAOYSA-N
Formula:	C7H7NO3
SMILES:	COc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	153.14
CAS:	100-17-4

Physical Properties

Property code	Value	Unit	Source
ea	0.87 ± 0.09	eV	NIST Webbook
ea	0.91 ± 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	9.00 ± 0.10	eV	NIST Webbook
ie	9.07	eV	NIST Webbook
ie	9.08 ± 0.01	eV	NIST Webbook

ie	8.60 ± 0.10	eV	NIST Webbook
ie	8.79	eV	NIST Webbook
log10ws	-2.41		Aqueous Solubility Prediction Method
log10ws	-2.41		Estimated Solubility Method
logp	1.603		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
pc	4010.84	kPa	Joback Method
rinpol	1414.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1424.30		NIST Webbook
tb	547.20	K	NIST Webbook
tc	811.60	K	Joback Method
tf	324.48	K	Aqueous Solubility Prediction Method
tf	327.10 ± 0.40	K	NIST Webbook
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.83	J/mol×K	811.60	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	242.84	J/mol×K	565.48	Joback Method
psub	5.78e-04	kPa	303.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range

psub	8.61e-04	kPa	307.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	1.41e-03	kPa	311.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	1.75e-03	kPa	313.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	2.79e-03	kPa	317.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	4.29e-03	kPa	321.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100174&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range:	https://www.doi.org/10.1016/j.tca.2010.11.034
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1453
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
psub:	Sublimation pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume