Benzene, 1-methoxy-2-nitro-

Other names:	1-Methoxy-2-nitrobenzene
	1-Nitro-2-methoxybenzene
	2-Methoxy-1-nitrobenzene
	2-Methoxynitrobenzene
	2-Nitroanisole
	Anisole, o-nitro-
	NCI-C60388
	UN 2730
	o-Nitro(methoxy)benzene
	o-Nitroanisole
	o-Nitrobenzene methyl ether
	o-Nitrophenyl methyl ether
Inchi:	InChI=1S/C7H7NO3/c1-11-7-5-3-2-4-6(7)8(9)10/h2-5H,1H3
InchiKey:	CFBYEGUGFPZCNF-UHFFFAOYSA-N
Formula:	C7H7NO3
SMILES:	COc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	153.14
CAS:	91-23-6

Physical Properties

Property code	Value	Unit	Source
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	9.04	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
log10ws	-1.96		Estimated Solubility Method
log10ws	-1.96		Aqueous Solubility Prediction Method
logp	1.603		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
pc	4010.84	kPa	Joback Method
rinpol	1367.70		NIST Webbook
rinpol	1367.70		NIST Webbook
rinpol	1296.00		NIST Webbook

tb	546.20	K	NIST Webbook
tc	811.60	K	Joback Method
tf	282.35 ± 0.50	K	NIST Webbook
tf	283.12	K	Aqueous Solubility Prediction Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.41	J/mol×K	770.58	Joback Method
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	297.83	J/mol×K	811.60	Joback Method
hvapt	58.60	kJ/mol	484.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58925e+01
Coeff. B	-5.84932e+03
Coeff. C	-3.03580e+01
Temperature range (K), min.	405.20
Temperature range (K), max.	583.17

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C91236&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume