Benzenamine, 2-methoxy-5-nitro-

Other names:	1-Amino-2-methoxy-5-nitrobenzene
	1-Methoxy-2-amino-4-nitrobenzene
	2-Amino-1-methoxy-4-nitrobenzene
	2-Amino-4-nitroanisole
	2-Methoxy-5-nitroaniline
	2-Methoxy-5-nitrobenzenamine
	3-Amino-4-methoxynitrobenzene
	3-Nitro-6-methoxyaniline
	4-Nitro-2-aminoanisole
	5-Nitro-2-methoxyaniline
	5-Nitro-o-anisidine
	Aniline, 2-methoxy-5-nitro-
	Azoamine Scarlet K
	Azoamine scarlet
	Azogene ecarlate R
	Azoic diazo component 13, base
	C.I. 37130
	C.I. Azoic diazo component 13
	Fast scarlet R
	NCI-C01934
	NSC 5510
	o-Anisidine nitrate
	o-Anisidine, 5-nitro-
Inchi:	InChI=1S/C7H8N2O3/c1-12-7-3-2-5(9(10)11)4-6(7)8/h2-4H,8H2,1H3
InchiKey:	NIPDVSLAMPAWTP-UHFFFAOYSA-N
Formula:	C7H8N2O3
SMILES:	COc1ccc([N+](=O)[O-])cc1N
Mol. weight [g/mol]:	168.15
CAS:	99-59-2

Physical Properties

Property code	Value	Unit	Source
chs	-3666.00 ± 0.58	kJ/mol	NIST Webbook
gf	98.21	kJ/mol	Joback Method
hf	-83.41	kJ/mol	Joback Method
hfs	-232.00	kJ/mol	NIST Webbook

hfus	24.89	kJ/mol	Joback Method
hvap	64.42	kJ/mol	Joback Method
log10ws	-3.17		Aqueous Solubility Prediction Method
logp	1.186		Crippen Method
mcvol	119.000	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
rinpol	1764.40		NIST Webbook
tb	642.99	K	Joback Method
tc	896.92	K	Joback Method
tf	390.82	K	Aqueous Solubility Prediction Method
vc	0.449	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.35	J/mol×K	642.99	Joback Method
cpg	301.87	J/mol×K	685.31	Joback Method
cpg	311.62	J/mol×K	727.63	Joback Method
cpg	320.60	J/mol×K	769.95	Joback Method
cpg	328.83	J/mol×K	812.28	Joback Method
cpg	336.32	J/mol×K	854.60	Joback Method
cpg	343.08	J/mol×K	896.92	Joback Method

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C99592&Units=SI

Legend

chs: Standard solid enthalpy of combustion

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume