Benzenamine, 3-methoxy-

Other names:	m-Anisidine
	m-Aminoanisole
	m-Anisylamine
	m-Methoxyaniline
	1-Amino-3-methoxybenzene
	3-Aminoanisole
	3-Methoxyaniline
	3-Methoxybenzenamine
	3-Anisidine
	3-Aminophenol methyl ether
	3-Methoxy-1-aminobenzene
	m-Aminomethoxybenzene
	NSC 7631
Inchi:	InChI=1S/C7H9NO/c1-9-7-4-2-3-6(8)5-7/h2-5H,8H2,1H3
InchiKey:	NCBZRJODKRCREW-UHFFFAOYSA-N
Formula:	C7H9NO
SMILES:	COc1cccc(N)c1
Mol. weight [g/mol]:	123.15
CAS:	536-90-3

Physical Properties

Property code	Value	Unit	Source
affp	913.00	kJ/mol	NIST Webbook
basg	881.10	kJ/mol	NIST Webbook
gf	72.29	kJ/mol	Joback Method
hf	-61.18	kJ/mol	Joback Method
hfus	13.92	kJ/mol	Joback Method
hvap	47.17	kJ/mol	Joback Method
ie	7.80 ± 0.10	eV	NIST Webbook
log10ws	-1.23		Crippen Method
logp	1.277		Crippen Method
mcvol	101.580	ml/mol	McGowan Method
pc	4249.61	kPa	Joback Method
rinpol	1229.00		NIST Webbook
rinpol	1198.10		NIST Webbook
rinpol	1229.00		NIST Webbook
rinpol	1229.00		NIST Webbook

ripol	2176.00		NIST Webbook
ripol	2176.00		NIST Webbook
tb	524.20	K	NIST Webbook
tc	711.90	K	Joback Method
tf	313.08	K	Joback Method
vc	0.366	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.54	J/mol×K	486.17	Joback Method
cpg	220.65	J/mol×K	523.79	Joback Method
cpg	231.16	J/mol×K	561.41	Joback Method
cpg	241.09	J/mol×K	599.03	Joback Method
cpg	250.46	J/mol×K	636.65	Joback Method
cpg	259.26	J/mol×K	674.27	Joback Method
cpg	267.51	J/mol×K	711.90	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C536903&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

affp: Proton affinity
basg: Gas basicity
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume