

Benzenamine, 2-methoxy-

Other names:	o-Anisidine o-Aminoanisole o-Methoxyaniline 1-Amino-2-methoxybenzene 2-Aminoanisole 2-Methoxy-1-aminobenzene 2-Methoxyaniline 2-Methoxybenzenamine 2-Anisidine o-Methoxyphenylamine o-Anisylamine 2-Methoxy-phenylamine o-Aminophenol methyl ether Ortho-anisidine 2-Aminomethoxybenzene NSC 3122
Inchi:	InChI=1S/C7H9NO/c1-9-7-5-3-2-4-6(7)8/h2-5H,8H2,1H3
InchiKey:	VMPITZXILSNTON-UHFFFAOYSA-N
Formula:	C7H9NO
SMILES:	<chem>COc1ccccc1N</chem>
Mol. weight [g/mol]:	123.15
CAS:	90-04-0

Physical Properties

Property code	Value	Unit	Source
affp	905.20	kJ/mol	NIST Webbook
basg	873.30	kJ/mol	NIST Webbook
chs	-3994.80 ± 1.30	kJ/mol	NIST Webbook
gf	72.29	kJ/mol	Joback Method
hf	-61.18	kJ/mol	Joback Method
hfs	-46.00	kJ/mol	NIST Webbook
hfus	13.92	kJ/mol	Joback Method
hvap	47.17	kJ/mol	Joback Method
ie	7.50 ± 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	1136.00		NIST Webbook
rinpol	1142.70		NIST Webbook
rinpol	1181.00		NIST Webbook
tb	498.15 ± 1.50	K	NIST Webbook
tb	497.20	K	NIST Webbook
tc	711.90	K	Joback Method
tf	313.08	K	Joback Method
vc	0.366	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.26	J/mol×K	674.27	Joback Method
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	267.51	J/mol×K	711.90	Joback Method
hvapt	57.50	kJ/mol	413.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90040&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
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
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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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