

Benzenamine, 2-methoxy-N,N-dimethyl-

Other names:	Benzene, 1-methoxy-2-dimethylamino- Benzene, 1-dimethylamino-2-methoxy- 2-Methoxy-N,N-dimethylaniline
Inchi:	InChI=1S/C9H13NO/c1-10(2)8-6-4-5-7-9(8)11-3/h4-7H,1-3H3
InchiKey:	XQFJDFIHJKPUEL-UHFFFAOYSA-N
Formula:	C9H13NO
SMILES:	<chem>COc1ccccc1N(C)C</chem>
Mol. weight [g/mol]:	151.21
CAS:	700-75-4

Physical Properties

Property code	Value	Unit	Source
gf	133.46	kJ/mol	Joback Method
hf	-68.72	kJ/mol	Joback Method
hfus	16.93	kJ/mol	Joback Method
hvap	43.02	kJ/mol	Joback Method
ie	7.59 ± 0.02	eV	NIST Webbook
log10ws	-1.50		Crippen Method
logp	1.761		Crippen Method
mcvol	129.760	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
rinpol	1213.00		NIST Webbook
rinpol	1213.00		NIST Webbook
tb	471.84	K	Joback Method
tc	676.27	K	Joback Method
tf	284.83	K	Joback Method
vc	0.468	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.72	J/mol×K	471.84	Joback Method
cpg	284.89	J/mol×K	505.91	Joback Method
cpg	298.34	J/mol×K	539.98	Joback Method

cpg	311.09	J/mol×K	574.05	Joback Method
cpg	323.14	J/mol×K	608.12	Joback Method
cpg	334.54	J/mol×K	642.20	Joback Method
cpg	345.28	J/mol×K	676.27	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C700754&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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