1,3-Benzenediamine, 4-methoxy-

Other names:	m-Phenylenediamine, 4-methoxy-
	C.I. Oxidation Base 12
	C.I. 76050
	Furro L
	Pelagol DA
	Pelagol Grey L
	Pelagol L
	1,3-Diamino-4-methoxybenzene
	2,4-Diaminoanisole
	4-Methoxy-m-phenylenediamine
	4-Methoxy-1,3-phenylenediamine
	Anisole, 2,4-diamino-
	2,4 DAA
	2,4-Diamineanisole
	2,4-Diaminoanisol
	2,4-Diaminoanisole base
	m-Diaminoanisole 1,3-diamino-4-methoxybenzene
	2,4-Diamino-1-methoxybenzene
	4-Methoxy-1,3-benzenediamine
	p-Methoxy-m-phenylenediamine
	4-MMPD
Inchi:	InChI=1S/C7H10N2O/c1-10-7-3-2-5(8)4-6(7)9/h2-4H,8-9H2,1H3
InchiKey:	BAHPQISAXRFLCL-UHFFFAOYSA-N
Formula:	C7H10N2O
SMILES:	COc1ccc(N)cc1N
Mol. weight [g/mol]:	138.17
CAS:	615-05-4

Physical Properties

Property code	Value	Unit	Source
gf	129.11	kJ/mol	Joback Method
hf	-38.86	kJ/mol	Joback Method
hfus	18.73	kJ/mol	Joback Method
hvap	58.47	kJ/mol	Joback Method
log10ws	-0.86		Crippen Method
logp	0.860		Crippen Method

mcvol	111.560	ml/mol	McGowan Method
pc	4492.23	kPa	Joback Method
tb	563.68	K	Joback Method
tc	800.40	K	Joback Method
tf	408.86	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.94	J/mol×K	563.68	Joback Method
cpg	269.93	J/mol×K	603.13	Joback Method
cpg	280.29	J/mol×K	642.59	Joback Method
cpg	290.02	J/mol×K	682.04	Joback Method
cpg	299.14	J/mol×K	721.49	Joback Method
cpg	307.64	J/mol×K	760.95	Joback Method
cpg	315.52	J/mol×K	800.40	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C615054&Units=SI

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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume