1,3-Benzenediamine, 4-methyl-

Other names:

1,3-Diamino-4-methylbenzene
1,3-benzenediamine, 4-methyl
2,4-Diamino-1-methylbenzene
2,4-Diamino-1-toluene
2,4-Diaminotoluen
2,4-Diaminotoluene
2,4-Diaminotoluol
2,4-Tolamine
2,4-Toluenediamine
2,4-Tolylenediamine
3-Amino-p-toluidine
4-Methyl-1,3-benzenediamine
4-Methyl-1,3-phenylenediamine
4-Methyl-m-phenylenediamine
4-m-Tolylenediamine
4-methyl-1,3-benzendiamine
5-Amino-o-toluidine
Benzofur MT
Brown for Fur T
C.I. Oxidation Base 35
C.I. Oxidation base 200
Developer 14
Developer B
Developer DB
Developer DBJ
Developer MC
Developer MT
Developer MT-CF
Developer MTD
Developer T
Eucanine GB
Fouramine J
Fourrine 94
Fourrine M
NCI-C02302
Nako TMT
Pelagol Grey J
Pelagol J
Pontamine Developer TN
Rcra waste number U221

	Renal MD
	TDA
	Tertral G
	Toluene-2,4-diamine
	Toluenediamine
	Tolylene-2,4-diamine
	UN 1709
	Zoba GKE
	Zogen developer H
	m-Toluenediamine
	m-Toluylendiamin
	m-Toluylenediamine
	m-Tolylenediamine
Inchi:	InChI=1S/C7H10N2/c1-5-2-3-6(8)4-7(5)9/h2-4H,8-9H2,1H3
InchiKey:	VOZKAJLKRJDJLL-UHFFFAOYSA-N
Formula:	C7H10N2
SMILES:	Cc1ccc(N)cc1N
Mol. weight [g/mol]:	122.17
CAS:	95-80-7

Physical Properties

Property code	Value	Unit	Source
gf	234.11	kJ/mol	Joback Method
hf	93.36	kJ/mol	Joback Method
hfus	17.54	kJ/mol	Joback Method
hvap	56.06	kJ/mol	Joback Method
log10ws	-1.21		Crippen Method
logp	1.159		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
pc	4596.38	kPa	Joback Method
tb	557.20	K	NIST Webbook
tb	565.20	K	NIST Webbook
tc	781.39	K	Joback Method
tf	386.63	K	Joback Method
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.29	J/mol×K	541.26	Joback Method
cpg	248.42	J/mol×K	581.28	Joback Method
cpg	258.84	J/mol×K	621.30	Joback Method
cpg	268.59	J/mol×K	661.32	Joback Method
cpg	277.69	J/mol×K	701.34	Joback Method
cpg	286.17	J/mol×K	741.37	Joback Method
cpg	294.05	J/mol×K	781.39	Joback Method
hvapt	67.70	kJ/mol	466.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	422.70	K	1.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55061e+01
Coeff. B	-5.08502e+03
Coeff. C	-9.01600e+01
Temperature range (K), min.	424.29
Temperature range (K), max.	588.95

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.89998e+01
Coeff. B	-1.15775e+04
Coeff. C	-8.54954e+00

Coeff. D	1.46401e-06
Temperature range (K), min.	371.25
Temperature range (K), max.	804.00

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1301.mol
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95807&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Densities and Viscosities of Diaminotoluene with Water, Ethanol, Propan-1-ol, and Butan-1-ol from (293.15 to 333.15) K:	https://www.doi.org/10.1021/je400968v
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1301
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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