1,4-Benzenediamine

Other names:

1,4-Diaminobenzene
1,4-Phenylenediamine
4-Aminoaniline
Aminogen II
BASF Ursol D
Benzofur D
C.I. 76060
C.I. Developer 13
C.I. Oxidation Base 10
Developer 13
Developer PF
Durafur Black R
Fenylenodwuamina
Fouramine D
Fourrine 1
Fourrine D
Fur Black 41867
Fur Brown 41866
Fur Yellow
Furro D
Futramine D
NSC 4777
Nako H
Orsin
Oxidation base 10
P-BENZENEDIAMINE
PARA
PPD
Paraphenylen-diamine
Pelagol D
Pelagol DR
Pelagol Grey D
Peltol D
Phenylenediamine, para
Renal PF
Rodol D
Santoflex IC
Santoflex LC
Tertral D
UN 1673

	USAF EK-394
	Ursol D
	Vulkanox 4020
	Zoba Black D
	p-Aminoaniline
	p-Diaminobenzene
	p-Fenylendiamin
	p-Phenylenediamine
Inchi:	InChI=1S/C6H8N2/c7-5-1-2-6(8)4-3-5/h1-4H,7-8H2
InchiKey:	CBCKQZAAMUWICA-UHFFFAOYSA-N
Formula:	C6H8N2
SMILES:	Nc1ccc(N)cc1
Mol. weight [g/mol]:	108.14
CAS:	106-50-3

Physical Properties

Property code	Value	Unit	Source
affp	905.90	kJ/mol	NIST Webbook
basg	874.00	kJ/mol	NIST Webbook
chs	-3511.00 ± 3.00	kJ/mol	NIST Webbook
chs	-3507.40 ± 0.63	kJ/mol	NIST Webbook
chs	-3509.30 ± 0.63	kJ/mol	NIST Webbook
gf	235.32	kJ/mol	Joback Method
hf	125.47	kJ/mol	Joback Method
hfs	6.30	kJ/mol	NIST Webbook
hfus	15.34	kJ/mol	Joback Method
hsub	92.20 ± 0.20	kJ/mol	NIST Webbook
hvap	53.17	kJ/mol	Joback Method
ie	7.16	eV	NIST Webbook
ie	7.15	eV	NIST Webbook
ie	7.34	eV	NIST Webbook
ie	7.61	eV	NIST Webbook
ie	7.34	eV	NIST Webbook
ie	6.87 ± 0.05	eV	NIST Webbook
ie	7.00 ± 0.10	eV	NIST Webbook
ie	6.84	eV	NIST Webbook
ie	6.89 ± 0.03	eV	NIST Webbook
ie	7.58	eV	NIST Webbook
log10ws	-0.38		Aqueous Solubility Prediction Method

logp	0.851		Crippen Method
mcvol	91.600	ml/mol	McGowan Method
pc	5374.91	kPa	Joback Method
rinpol	212.86		NIST Webbook
ss	149.70	J/mol×K	NIST Webbook
tb	540.20	K	NIST Webbook
tc	757.17	K	Joback Method
tf	412.30 ± 0.50	K	NIST Webbook
tf	415.70 ± 0.10	K	NIST Webbook
tf	414.20 ± 0.20	K	NIST Webbook
tf	414.14 ± 0.30	K	NIST Webbook
tf	414.35 ± 0.20	K	NIST Webbook
vc	0.322	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.73	J/mol×K	594.66	Joback Method
cpg	224.60	J/mol×K	635.29	Joback Method
cpg	232.82	J/mol×K	675.91	Joback Method
cpg	240.43	J/mol×K	716.54	Joback Method
cpg	195.92	J/mol×K	513.40	Joback Method
cpg	206.18	J/mol×K	554.03	Joback Method
cpg	247.46	J/mol×K	757.17	Joback Method
cps	155.64	J/mol×K	300.00	NIST Webbook
hfust	24.90	kJ/mol	416.00	NIST Webbook
hfust	21.70	kJ/mol	412.30	NIST Webbook
hfust	21.70	kJ/mol	412.30	NIST Webbook
sfust	59.80	J/mol×K	416.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53683e+01
Coeff. B	-4.78156e+03
Coeff. C	-9.54010e+01

Temperature range (K), min.	412.47
Temperature range (K), max.	570.86

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.17201e+02
Coeff. B	-1.32852e+04
Coeff. C	-1.41926e+01
Coeff. D	4.47876e-06
Temperature range (K), min.	413.00
Temperature range (K), max.	796.00

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol1295.mol

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C106503&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1295

Legend

affp: Proton affinity

basg: Gas basicity

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

cps: Solid phase 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

hfust: Enthalpy of fusion at a given temperature

hsub: Enthalpy of sublimation 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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume