1,2-Benzenediamine

Other names: 1,2-Diaminobenzene
1,2-Fenylendiamin
1,2-Phenylenediamine
2-Aminoaniline
C.I. 76010
C.I. Oxidation Base 16
EK 1700
IK 3
NSC 5354
O-BENZENEDIAMINE
OPDA
Orthamine
PODA
SQ 15500
benzene, 1,2-diamino-
o-Aminoaniline
o-Diaminobenzene
o-Fenylendiamin
o-Phenylenediamine
o-aminophenylamine

Inchi: InChI=1S/C6H8N2/c7-5-3-1-2-4-6(5)8/h1-4H,7-8H2
InchiKey: GEYOCULIXLDCMW-UHFFFAOYSA-N
Formula: C6H8N2
SMILES: Nc1ccccc1N
Mol. weight [g/mol]: 108.14
CAS: 95-54-5

Physical Properties

Property code	Value	Unit	Source
affp	896.50	kJ/mol	NIST Webbook
basg	865.80	kJ/mol	NIST Webbook
chs	-3504.00 ± 3.00	kJ/mol	NIST Webbook
chs	-3543.50 ± 5.70	kJ/mol	NIST Webbook
gf	235.32	kJ/mol	Joback Method
hf	125.47	kJ/mol	Joback Method
hfs	39.10 ± 5.70	kJ/mol	NIST Webbook
hfs	0.00	kJ/mol	NIST Webbook

hfus	15.34	kJ/mol	Joback Method
hsub	85.50 ± 0.30	kJ/mol	NIST Webbook
hvap	53.17	kJ/mol	Joback Method
ie	7.40 ± 0.10	eV	NIST Webbook
ie	7.69	eV	NIST Webbook
ie	7.78	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
ie	7.36	eV	NIST Webbook
ie	7.20	eV	NIST Webbook
ie	7.45	eV	NIST Webbook
log10ws	-0.42		Aqueous Solubility Prediction Method
logp	0.851		Crippen Method
mcvol	91.600	ml/mol	McGowan Method
pc	5374.91	kPa	Joback Method
ss	152.09	J/mol×K	NIST Webbook
tb	530.15 ± 2.00	K	NIST Webbook
tb	460.20 ± 1.00	K	NIST Webbook
tb	530.20	K	NIST Webbook
tc	757.17	K	Joback Method
tf	374.90	K	Aqueous Solubility Prediction Method
tf	373.90 ± 0.50	K	NIST Webbook
tf	377.00 ± 0.20	K	NIST Webbook
vc	0.322	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.92	J/mol×K	513.40	Joback Method
cpg	240.43	J/mol×K	716.54	Joback Method
cpg	232.82	J/mol×K	675.91	Joback Method
cpg	224.60	J/mol×K	635.29	Joback Method
cpg	215.73	J/mol×K	594.66	Joback Method
cpg	206.18	J/mol×K	554.03	Joback Method
cpg	247.46	J/mol×K	757.17	Joback Method
cps	162.13	J/mol×K	300.00	NIST Webbook
cps	150.82	J/mol×K	298.15	NIST Webbook
hfust	23.10	kJ/mol	373.90	NIST Webbook
hfust	23.10	kJ/mol	373.90	NIST Webbook
hfust	23.10	kJ/mol	373.85	NIST Webbook
sfust	62.00	J/mol×K	373.85	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51586e+01
Coeff. B	-4.67140e+03
Coeff. C	-8.70030e+01
Temperature range (K), min.	376.95
Temperature range (K), max.	561.40

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.04531e+02
Coeff. B	-1.20767e+04
Coeff. C	-1.24573e+01
Coeff. D	4.01984e-06
Temperature range (K), min.	376.95
Temperature range (K), max.	781.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1293
Solubility determination and correlation for o-phenylenediamine in (methanol, ethanol, acetonitrile and water) and their binary solvents from T = (283.15-318.15) K:	https://www.doi.org/10.1016/j.jct.2016.10.018
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1293.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95545&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
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