1,4-Benzenediamine, N-phenyl-

Other names:
1,4-Benzenediamine, N1-phenyl-
4-(Phenylamino)aniline
4-Aminodiphenylamine
Acna Black DF Base
Azosalt R
C.I. 37240
C.I. 76085
C.I. Azoic Diazo Component 22
C.I. Developer 15
C.I. Oxidation Base 2
Diphenyl Black
Diphenylamine, 4-amino-
Diphenylamine, p-amino-
Fast Blue R Salt
Luxan Black R
N-(4-Aminophenyl)aniline
N-4'-Bianiline
N-Fenyl-p-fenylendiamin
N-Phenyl-1,4-benzenediamine
N-Phenyl-1,4-phenylenediamine
N-Phenyl-p-aminoaniline
N-Phenyl-p-phenylenediamine
NCI-C02233
NSC 3401
Naphthoelan Navy Blue
Oxy Acid Black Base
Peltol BR
Peltol BR II
Semidin
Semidine
UBOB
Variamine Blue RT
Variamine Blue Salt RT
p-(Phenylamino)aniline
p-Aminodifenylamin
p-Aminodiphenylamine
p-Anilinoaniline
p-Phenylenediamine, N-phenyl-
p-Semidine

Inchi: InChI=1S/C12H12N2/c13-10-6-8-12(9-7-10)14-11-4-2-1-3-5-11/h1-9,14H,13H2

InchiKey: ATGUVEKSASEFFO-UHFFFAOYSA-N
Formula: C12H12N2
SMILES: Nc1ccc(Nc2ccccc2)cc1
Mol. weight [g/mol]: 184.24
CAS: 101-54-2

Physical Properties

Property code	Value	Unit	Source
gf	421.19	kJ/mol	Joback Method
hf	257.84	kJ/mol	Joback Method
hfus	24.82	kJ/mol	Joback Method
hvap	64.60	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	3.012		Crippen Method
mcvol	152.380	ml/mol	McGowan Method
pc	3659.77	kPa	Joback Method
tb	627.00	K	NIST Webbook
tc	910.40	K	Joback Method
tf	339.00	K	NIST Webbook
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.08	J/mol×K	655.00	Joback Method
cpg	398.63	J/mol×K	697.57	Joback Method
cpg	411.93	J/mol×K	740.13	Joback Method
cpg	424.08	J/mol×K	782.70	Joback Method
cpg	435.16	J/mol×K	825.27	Joback Method
cpg	445.25	J/mol×K	867.84	Joback Method
cpg	454.44	J/mol×K	910.40	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	428.00	K	0.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56513e+01
Coeff. B	-5.80754e+03
Coeff. C	-1.00620e+02
Temperature range (K), min.	478.62
Temperature range (K), max.	662.29

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C101542&Units=SI

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

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

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

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