

Benzidine

Other names:	4,4'-Bianiline 4,4'-Biphenyldiamine 4,4'-Biphenylenediamine 4,4'-Diamino-1,1'-biphenyl 4,4'-Diaminobiphenyl 4,4'-Diaminodiphenyl 4,4'-Diphenylenediamine Benzidin Benzidina Benzydyna Biphenyl -4,4'-ylenediamine Biphenyl,4,4'-diamino- C.I. 37225 C.I. Azoic Diazo Component 112 Fast Corinth Base B NCI-C03361 NSC 146476 Rcra waste number U021 UN 1885 [1,1'-Biphenyl]-4,4'-diamine p,p'-Bianiline p,p'-Diaminobiphenyl p,p'-Dianiline p,p-Bianiline p-Diaminodiphenyl p-benzidine
Inchi:	InChI=1S/C12H12N2/c13-11-5-1-9(2-6-11)10-3-7-12(14)8-4-10/h1-8H,13-14H2
InchiKey:	HFACYLZERDEVSX-UHFFFAOYSA-N
Formula:	C12H12N2
SMILES:	<chem>Nc1ccc(-c2ccc(N)cc2)cc1</chem>
Mol. weight [g/mol]:	184.24
CAS:	92-87-5

Physical Properties

Property code	Value	Unit	Source
chs	-6544.20	kJ/mol	NIST Webbook

chs	-6508.00 ± 1.00		kJ/mol	NIST Webbook
gf	388.62		kJ/mol	Joback Method
hf	226.69		kJ/mol	Joback Method
hfs	107.00		kJ/mol	NIST Webbook
hfus	24.53		kJ/mol	Joback Method
hvap	69.46		kJ/mol	Joback Method
ie	6.88		eV	NIST Webbook
log10ws	-2.70			Aqueous Solubility Prediction Method
log10ws	-2.70			Estimated Solubility Method
logp	2.518			Crippen Method
mcvol	152.380		ml/mol	McGowan Method
pc	3791.65		kPa	Joback Method
rinpol	2070.00			NIST Webbook
rinpol	2042.00			NIST Webbook
rinpol	2111.00			NIST Webbook
rinpol	2042.00			NIST Webbook
rinpol	2111.00			NIST Webbook
tb	682.34		K	Joback Method
tc	947.66		K	Joback Method
tf	273.15 ± 2.00		K	NIST Webbook
tf	400.00 ± 1.00		K	NIST Webbook
vc	0.549		m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.10	J/mol×K	682.34	Joback Method
cpg	404.97	J/mol×K	726.56	Joback Method
cpg	417.65	J/mol×K	770.78	Joback Method
cpg	429.21	J/mol×K	815.00	Joback Method
cpg	439.73	J/mol×K	859.22	Joback Method
cpg	449.29	J/mol×K	903.44	Joback Method
cpg	457.98	J/mol×K	947.66	Joback Method
hfust	19.10	kJ/mol	400.20	NIST Webbook
hfust	19.10	kJ/mol	400.20	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	673.20	K	98.70	NIST Webbook

Sources

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

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C92875&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas 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
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
rinpol:	Non-polar retention indices
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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