

2-Aminobiphenyl

Other names:	[1,1'-Biphenyl]-2-amine 2-Biphenylamine o-Aminobiphenyl o-Aminodiphenyl o-Biphenylamine o-Phenylaniline 2-Aminodiphenyl 2-Phenylaniline o-Xenylamine 2-Aminobifenyyl 2-Phenylbenzenamine 2-Amino-1,1'-biphenyl NSC 7661 biphenyl-2-ylamine
Inchi:	InChI=1S/C12H11N/c13-12-9-5-4-8-11(12)10-6-2-1-3-7-10/h1-9H,13H2
InchiKey:	TWBPWBPGNQWFSJ-UHFFFAOYSA-N
Formula:	C12H11N
SMILES:	Nc1ccccc1-c1ccccc1
Mol. weight [g/mol]:	169.22
CAS:	90-41-5

Physical Properties

Property code	Value	Unit	Source
chs	-6387.97 ± 0.88	kJ/mol	NIST Webbook
chs	-6406.16	kJ/mol	NIST Webbook
gf	331.80	kJ/mol	Joback Method
hf	184.41 ± 0.54	kJ/mol	NIST Webbook
hfs	93.80 ± 1.10	kJ/mol	NIST Webbook
hfus	19.73	kJ/mol	Joback Method
hsub	90.60	kJ/mol	NIST Webbook
hvap	58.16	kJ/mol	Joback Method
ie	7.28 ± 0.02	eV	NIST Webbook
ie	7.60 ± 0.10	eV	NIST Webbook
log10ws	-3.71		Crippen Method
logp	2.936		Crippen Method
mcvol	142.400	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method

rinpol	271.35		NIST Webbook
rinpol	273.63		NIST Webbook
rinpol	273.12		NIST Webbook
rinpol	1534.00		NIST Webbook
rinpol	1584.00		NIST Webbook
rinpol	1598.00		NIST Webbook
rinpol	273.12		NIST Webbook
rinpol	1584.00		NIST Webbook
rinpol	1598.00		NIST Webbook
ss	233.48	J/molxK	NIST Webbook
tb	572.20	K	NIST Webbook
tb	572.00	K	NIST Webbook
tc	863.82	K	Joback Method
tf	322.50 ± 0.50	K	NIST Webbook
tf	322.65 ± 1.50	K	NIST Webbook
tt	322.28 ± 0.02	K	NIST Webbook
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.49	J/molxK	734.32	Joback Method
cpg	350.95	J/molxK	647.99	Joback Method
cpg	364.81	J/molxK	691.16	Joback Method
cpg	409.23	J/molxK	863.82	Joback Method
cpg	399.61	J/molxK	820.65	Joback Method
cpg	389.06	J/molxK	777.49	Joback Method
cpg	335.82	J/molxK	604.83	Joback Method
cps	221.86	J/molxK	298.15	NIST Webbook
hfust	13.99	kJ/mol	322.30	NIST Webbook
hfust	13.99	kJ/mol	322.30	NIST Webbook
hvapt	51.70	kJ/mol	481.50	NIST Webbook
hvapt	55.20	kJ/mol	481.50	NIST Webbook
hvapt	58.50	kJ/mol	481.50	NIST Webbook
hvapt	61.80	kJ/mol	481.50	NIST Webbook
hvapt	65.10	kJ/mol	481.50	NIST Webbook
hvapt	68.60	kJ/mol	481.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	443.20	K	2.00	NIST Webbook
tbrp	443.00	K	2.00	NIST Webbook
tbrp	419.50 ± 1.50	K	0.70	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90415&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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