[1,1'-Biphenyl]-4-amine

Other names: (1,1'-Biphenyl-4-yl)amine
4-Amino-1,1'-biphenyl
4-Aminobifenyl
4-Aminobiphenyl
4-Aminodifenil
4-Aminodiphenyl
4-Bifenylamin
4-Biphenylamine
4-Biphenylylamine
4-Phenylaniline
Aniline, p-phenyl-
Biphenyl-4-ylamine
Biphenylamine
NSC 7660
Paraaminodiphenyl
Xenylamin
Xenylamine
p-Aminobiphenyl
p-Aminodiphenyl
p-Biphenylamine
p-Phenylaniline
p-Xenylamine

Inchi: InChI=1S/C12H11N/c13-12-8-6-11(7-9-12)10-4-2-1-3-5-10/h1-9H,13H2

InchiKey: DMVOXQPQNTYEKQ-UHFFFAOYSA-N

Formula: C12H11N

SMILES: Nc1ccc(-c2ccccc2)cc1

Mol. weight [g/mol]: 169.22

CAS: 92-67-1

Physical Properties

Property code	Value	Unit	Source
chs	-6375.50	kJ/mol	NIST Webbook
gf	331.80	kJ/mol	Joback Method
hf	204.37	kJ/mol	Joback Method
hfus	19.73	kJ/mol	Joback Method
hvap	58.16	kJ/mol	Joback Method

ie	7.50 ± 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	295.26		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1683.00		NIST Webbook
rinpol	294.70		NIST Webbook
rinpol	298.05		NIST Webbook
rinpol	293.92		NIST Webbook
ripol	2636.00		NIST Webbook
ripol	2636.00		NIST Webbook
tb	575.20	K	NIST Webbook
tb	575.00	K	NIST Webbook
tc	863.82	K	Joback Method
tf	324.15 ± 0.60	K	NIST Webbook
tf	326.35 ± 0.35	K	NIST Webbook
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.82	J/mol×K	604.83	Joback Method
cpg	350.95	J/mol×K	647.99	Joback Method
cpg	364.81	J/mol×K	691.16	Joback Method
cpg	377.49	J/mol×K	734.32	Joback Method
cpg	389.06	J/mol×K	777.49	Joback Method
cpg	399.61	J/mol×K	820.65	Joback Method
cpg	409.23	J/mol×K	863.82	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	464.20	K	2.00	NIST Webbook
tbrp	464.00	K	2.00	NIST Webbook
tbrp	439.00	K	0.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.71355e+01
Coeff. B	-6.11546e+03
Coeff. C	-8.66360e+01
Temperature range (K), min.	449.62
Temperature range (K), max.	603.84

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92671&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hfus:	Enthalpy of fusion 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
ripol:	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