1,1'-Biphenyl, 4-nitro-

Other names:	1-Nitro-4-phenylbenzene
	4-Nitrodiphenyl
	4-Phenylnitrobenzene
	4-nitro-1,1'-biphenyl
	4-nitrobiphenyl
	Ba 2794
	NSC 1324
	PNB
	biphenyl, 4-nitro-
	p-Nitrobiphenyl
	p-Nitrodiphenyl
	p-Phenylnitrobenzene
Inchi:	InChI=1S/C12H9NO2/c14-13(15)12-8-6-11(7-9-12)10-4-2-1-3-5-10/h1-9H
InchiKey:	BAJQRLZAPXASRD-UHFFFAOYSA-N
Formula:	C12H9NO2
SMILES:	O=[N+]([O-])c1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	199.21
CAS:	92-93-3

Physical Properties

Property code	Value	Unit	Source
chs	-6048.80 ± 6.30	kJ/mol	NIST Webbook
ea	1.20 ± 0.10	eV	NIST Webbook
gf	300.90	kJ/mol	Joback Method
hf	159.82	kJ/mol	Joback Method
hfus	25.89	kJ/mol	Joback Method
hvap	64.11	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	3.262		Crippen Method
mcvol	149.840	ml/mol	McGowan Method
pc	3415.86	kPa	Joback Method
rinpol	1856.00		NIST Webbook
rinpol	1834.00		NIST Webbook
rinpol	313.20		NIST Webbook
rinpol	312.68		NIST Webbook
rinpol	312.72		NIST Webbook
rinpol	313.14		NIST Webbook

rinpol	1816.00		NIST Webbook
rinpol	314.59		NIST Webbook
rinpol	312.30		NIST Webbook
rinpol	1839.00		NIST Webbook
rinpol	314.59		NIST Webbook
rinpol	1834.00		NIST Webbook
rinpol	312.30		NIST Webbook
rinpol	1839.00		NIST Webbook
rinpol	1832.00		NIST Webbook
rinpol	1834.00		NIST Webbook
rinpol	313.20		NIST Webbook
rinpol	313.35		NIST Webbook
tb	684.14	K	Joback Method
tc	959.45	K	Joback Method
tf	433.97	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.07	J/mol×K	959.45	Joback Method
cpg	387.39	J/mol×K	730.02	Joback Method
cpg	399.76	J/mol×K	775.91	Joback Method
cpg	410.91	J/mol×K	821.79	Joback Method
cpg	420.94	J/mol×K	867.68	Joback Method
cpg	429.96	J/mol×K	913.56	Joback Method
cpg	373.70	J/mol×K	684.14	Joback Method
psub	5.00e-05	kPa	323.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	1.58e-04	kPa	333.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range

psub	4.85e-04	kPa	343.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	1.41e-03	kPa	353.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	3.72e-03	kPa	363.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	0.02	kPa	380.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	497.20	K	4.00	NIST Webbook

Sources

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=C92933&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range:	https://www.doi.org/10.1016/j.tca.2010.11.034

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
ea:	Electron affinity
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
psub:	Sublimation 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