1,1'-Biphenyl, 2-nitro-

Other names:	Biphenyl, 2-nitro-
	o-Nitrobiphenyl
	o-Nitrodiphenyl
	Onb
	2-Nitrobiphenyl
	2-Nitrodiphenyl
Inchi:	InChI=1S/C12H9NO2/c14-13(15)12-9-5-4-8-11(12)10-6-2-1-3-7-10/h1-9H
InchiKey:	YOJKKXRJMXIKSR-UHFFFAOYSA-N
Formula:	C12H9NO2
SMILES:	O=[N+]([O-])c1ccccc1-c1ccccc1
Mol. weight [g/mol]:	199.21
CAS:	86-00-0

Physical Properties

Property code	Value	Unit	Source
ea	1.07 ± 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	1669.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1698.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1686.00		NIST Webbook
rinpol	1696.33		NIST Webbook
rinpol	290.25		NIST Webbook
rinpol	288.70		NIST Webbook
rinpol	288.56		NIST Webbook
rinpol	284.73		NIST Webbook

rinpol	288.54		NIST Webbook
rinpol	287.61		NIST Webbook
rinpol	290.25		NIST Webbook
rinpol	285.80		NIST Webbook
rinpol	285.80		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1686.00		NIST Webbook
rinpol	1691.22		NIST Webbook
tb	593.20	K	NIST Webbook
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	373.70	J/mol×K	684.14	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	438.07	J/mol×K	959.45	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	440.70	K	1.70	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C86000&Units=SI

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
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
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