1,1'-Biphenyl, 3-nitro-

Other names:	Biphenyl, 3-nitro- m-Nitrobiphenyl 3-Nitrobiphenyl m-Nitrodiphenyl 3-Nitro-1,1'-biphenyl
Inchi:	InChI=1S/C12H9NO2/c14-13(15)12-8-4-7-11(9-12)10-5-2-1-3-6-10/h1-9H
InchiKey:	FYRPEHRWMVMHQM-UHFFFAOYSA-N
Formula:	C12H9NO2
SMILES:	O=[N+]([O-])c1cccc(-c2ccccc2)c1
Mol. weight [g/mol]:	199.21
CAS:	2113-58-8

Physical Properties

Property code	Value	Unit	Source
chs	-6073.50 ± 6.30	kJ/mol	NIST Webbook
ea	1.12 ± 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	308.47		NIST Webbook
rinpol	1802.00		NIST Webbook
rinpol	1813.00		NIST Webbook
rinpol	1808.00		NIST Webbook
rinpol	307.90		NIST Webbook
rinpol	308.30		NIST Webbook
rinpol	308.70		NIST Webbook
rinpol	308.75		NIST Webbook
rinpol	310.09		NIST Webbook
rinpol	307.70		NIST Webbook
rinpol	1792.00		NIST Webbook
rinpol	1831.00		NIST Webbook
rinpol	1792.00		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	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	416.20	K	1.00	NIST Webbook
tbrp	432.00 ± 3.00	K	0.10	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2113588&Units=SI

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
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

Latest version available from:
https://www.chemeo.com/cid/65-511-2/1-1-Biphenyl-3-nitro.pdf
Generated by Cheméo on 2024-04-19 16:11:05.690862936 +0000 UTC m=+15832314.611440257.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.