1,1'-Biphenyl, 3-chloro-

Other names:	1,1'-Biphenyl, 3-monochloro-
	1-chloro-3-phenylbenzene
	3-Chloro-1,1'-biphenyl
	3-Chlorobiphenyl
	3-Chlorodiphenyl
	3-Monochlorobiphenyl
	Biphenyl, 3-chloro-
	PCB 2
	m-Chlorobiphenyl
	m-Chlorodiphenyl
Inchi:	InChI=1S/C12H9Cl/c13-12-8-4-7-11(9-12)10-5-2-1-3-6-10/h1-9H
InchiKey:	NMWSKOLWZZWHPL-UHFFFAOYSA-N
Formula:	C12H9Cl
SMILES:	Clc1cccc(-c2ccccc2)c1
Mol. weight [g/mol]:	188.66

Physical Properties

Property code	Value	Unit	Source
af	0.3669		Cheméo Relay (1.0)
chl	-6045.96	kJ/mol	NIST Webbook
gf	253.42	kJ/mol	Joback Method
hf	166.81	kJ/mol	Cheméo Relay (1.0)
hfus	18.73	kJ/mol	Joback Method
hvap	74.30 ± 1.10	kJ/mol	NIST Webbook
ie	8.36	eV	Cheméo Relay (1.0)
log10ws	-4.88		Aqueous Solubility Prediction Method
log10ws	-4.88		Estimated Solubility Method
logp	4.007		Crippen Method
mcvol	144.660	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
rinpol	1554.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1575.00		NIST Webbook
rinpol	1567.10		NIST Webbook
rinpol	1571.40		NIST Webbook

rinpol	1575.70		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1548.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1548.00		NIST Webbook
rinpol	1560.00		NIST Webbook
tb	557.70	K	NIST Webbook
tc	800.50	K	Cheméo Relay (1.0)
tf	295.18	K	Cheméo Relay (1.0)
vc	0.538	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.46	J/mol×K	739.92	Joback Method
cpg	376.10	J/mol×K	825.02	Joback Method
cpg	366.74	J/mol×K	782.47	Joback Method
cpg	345.19	J/mol×K	697.37	Joback Method
cpg	304.63	J/mol×K	569.73	Joback Method
cpg	319.35	J/mol×K	612.28	Joback Method
cpg	332.84	J/mol×K	654.83	Joback Method
dvisc	0.0018784	Pa×s	320.28	Joback Method
dvisc	0.0010478	Pa×s	361.86	Joback Method
dvisc	0.0006592	Pa×s	403.43	Joback Method
dvisc	0.0004522	Pa×s	445.00	Joback Method
dvisc	0.0003309	Pa×s	486.58	Joback Method
dvisc	0.0002543	Pa×s	528.15	Joback Method
dvisc	0.0002031	Pa×s	569.73	Joback Method
hvapt	66.00	kJ/mol	494.00	NIST Webbook
hvapt	66.20	kJ/mol	334.50	NIST Webbook
hvapt	66.60	kJ/mol	368.00	NIST Webbook
hvapt	69.20	kJ/mol	371.50	NIST Webbook

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2051618&Units=SI

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume