

1,1'-Biphenyl, 2,2',4,5,5'-pentachloro-

Other names:	1,2,4-trichloro-5-(2,5-dichlorophenyl)benzene 2,2',4,5,5'-Pentachloro-1,1'-biphenyl 2,2',4,5,5'-Pentachlorobiphenyl PCB 101
Inchi:	InChI=1S/C12H5Cl5/c13-6-1-2-9(14)7(3-6)8-4-11(16)12(17)5-10(8)15/h1-5H
InchiKey:	LAHWLEDBADHJGA-UHFFFAOYSA-N
Formula:	C12H5Cl5
SMILES:	Clc1ccc(Cl)c(-c2cc(Cl)c(Cl)cc2Cl)c1
Mol. weight [g/mol]:	326.43
CAS:	37680-73-2

Physical Properties

Property code	Value	Unit	Source
gf	167.18	kJ/mol	Joback Method
hf	46.00	kJ/mol	Joback Method
hfus	33.96	kJ/mol	Joback Method
hvap	72.09	kJ/mol	Joback Method
log10ws	-7.53		Aqueous Solubility Prediction Method
logp	6.621		Crippen Method
mcvol	193.620	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	2082.20		NIST Webbook
rinpol	2082.20		NIST Webbook
rinpol	2134.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2134.00		NIST Webbook
rinpol	2134.00		NIST Webbook
rinpol	2134.00		NIST Webbook
rinpol	2134.00		NIST Webbook
rinpol	2135.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2132.00		NIST Webbook
rinpol	2134.00		NIST Webbook
tb	739.37	K	Joback Method
tc	1008.22	K	Joback Method
tf	350.10 ± 0.20	K	NIST Webbook
vc	0.737	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.09	J/molxK	963.41	Joback Method
cpg	428.46	J/molxK	1008.22	Joback Method
cpg	385.50	J/molxK	739.37	Joback Method
cpg	394.64	J/molxK	784.18	Joback Method
cpg	402.91	J/molxK	828.99	Joback Method
cpg	410.38	J/molxK	873.79	Joback Method
cpg	417.08	J/molxK	918.60	Joback Method
dvisc	0.0001570	Paxs	739.37	Joback Method
dvisc	0.0001860	Paxs	697.82	Joback Method
dvisc	0.0006694	Paxs	490.04	Joback Method
dvisc	0.0004783	Paxs	531.60	Joback Method
dvisc	0.0003588	Paxs	573.15	Joback Method
dvisc	0.0002798	Paxs	614.71	Joback Method
dvisc	0.0002252	Paxs	656.26	Joback Method
hfust	18.80	kJ/mol	350.10	NIST Webbook
hfust	18.80	kJ/mol	350.10	NIST Webbook
hsubt	92.70	kJ/mol	308.00	NIST Webbook
hvapt	83.70	kJ/mol	398.00	NIST Webbook
hvapt	86.40	kJ/mol	368.00	NIST Webbook

Sources

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method:

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C37680732&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
hvac:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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

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