

1,1'-Biphenyl, 3,3'-dichloro-

Other names:	1-chloro-3-(3-chlorophenyl)benzene 3,3'-Dichlorobiphenyl 3,3'-Dichlorodiphenyl Biphenyl, 3,3'-dichloro- PCB 11 m,m'-Dichlorobiphenyl
Inchi:	InChI=1S/C12H8Cl2/c13-11-5-1-3-9(7-11)10-4-2-6-12(14)8-10/h1-8H
InchiKey:	KTXUOWUHFLBZPW-UHFFFAOYSA-N
Formula:	C12H8Cl2
SMILES:	Clc1cccc(-c2cccc(Cl)c2)c1
Mol. weight [g/mol]:	223.10
CAS:	2050-67-1

Physical Properties

Property code	Value	Unit	Source
gf	231.86	kJ/mol	Joback Method
hf	127.63	kJ/mol	Joback Method
hfus	22.53	kJ/mol	Joback Method
hvap	81.00 ± 0.20	kJ/mol	NIST Webbook
log10ws	-5.80		Aqueous Solubility Prediction Method
logp	4.660		Crippen Method
mcvol	156.900	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	1725.40		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1725.40		NIST Webbook
rinpol	1746.00		NIST Webbook
rinpol	1756.00		NIST Webbook
rinpol	1769.00		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	1769.00		NIST Webbook
tb	612.14	K	Joback Method
tc	871.88	K	Joback Method
tf	362.72	K	Joback Method
vc	0.590	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.60	J/molxK	871.88	Joback Method
cpg	383.35	J/molxK	828.59	Joback Method
cpg	374.26	J/molxK	785.30	Joback Method
cpg	364.26	J/molxK	742.01	Joback Method
cpg	353.28	J/molxK	698.72	Joback Method
cpg	341.24	J/molxK	655.43	Joback Method
cpg	328.07	J/molxK	612.14	Joback Method
dvisc	0.0013975	Paxs	362.72	Joback Method
dvisc	0.0001963	Paxs	612.14	Joback Method
dvisc	0.0002417	Paxs	570.57	Joback Method
dvisc	0.0003074	Paxs	529.00	Joback Method
dvisc	0.0004074	Paxs	487.43	Joback Method
dvisc	0.0005691	Paxs	445.86	Joback Method
dvisc	0.0008516	Paxs	404.29	Joback Method
hvapt	75.40	kJ/mol	368.00	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2050671&Units=SI>

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

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>

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

h_{vap}:	Enthalpy of vaporization at standard conditions
h_{vapt}:	Enthalpy of vaporization at a given temperature
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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