

1,1'-Biphenyl, 3,4,4'-trichloro-

Other names:	3,4,4'-Trichlorobiphenyl
	PCB 37
Inchi:	InChI=1S/C12H7Cl3/c13-10-4-1-8(2-5-10)9-3-6-11(14)12(15)7-9/h1-7H
InchiKey:	YZANRISAORXTHU-UHFFFAOYSA-N
Formula:	C12H7Cl3
SMILES:	Clc1ccc(-c2ccc(Cl)c(Cl)c2)cc1
Mol. weight [g/mol]:	257.55

Physical Properties

Property code	Value	Unit	Source
hf	105.25	kJ/mol	Cheméo Relay (1.0)
hfus	26.34	kJ/mol	Joback Method
hvap	90.76	kJ/mol	Cheméo Relay (1.0)
ie	8.32	eV	Cheméo Relay (1.0)
log10ws	-7.06		Aqueous Solubility Prediction Method
logp	5.314		Crippen Method
mcvol	169.140	ml/mol	McGowan Method
rinpol	1980.00		NIST Webbook
rinpol	2005.00		NIST Webbook
rinpol	1980.00		NIST Webbook
tb	612.49	K	Cheméo Relay (1.0)
tf	345.59	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.20	J/mol×K	654.55	Joback Method
cpg	405.36	J/mol×K	917.95	Joback Method
cpg	398.13	J/mol×K	874.05	Joback Method
cpg	390.14	J/mol×K	830.15	Joback Method
cpg	381.33	J/mol×K	786.25	Joback Method
cpg	371.61	J/mol×K	742.35	Joback Method
cpg	360.92	J/mol×K	698.45	Joback Method

dvisc	0.0003625	Pa×s	529.86	Joback Method
dvisc	0.0001852	Pa×s	654.55	Joback Method
dvisc	0.0002248	Pa×s	612.99	Joback Method
dvisc	0.0002805	Pa×s	571.42	Joback Method
dvisc	0.0010725	Pa×s	405.16	Joback Method
dvisc	0.0004893	Pa×s	488.29	Joback Method
dvisc	0.0006985	Pa×s	446.73	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C38444905&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):

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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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