3,3',4-Trichloro-1,1'-biphenyl

Other names:	1,1'-Biphenyl, 3,3',4-trichloro
	3,3',4-Trichlorobiphenyl
	PCB 35
Inchi:	InChI=1S/C12H7Cl3/c13-10-3-1-2-8(6-10)9-4-5-11(14)12(15)7-9/h1-7H
InchiKey:	JHBVPKZLIBDTJR-UHFFFAOYSA-N
Formula:	C12H7Cl3
SMILES:	Clc1cccc(-c2ccc(Cl)c(Cl)c2)c1
Mol. weight [g/mol]:	257.54
CAS:	37680-69-6

Physical Properties

Property code	Value	Unit	Source
gf	210.30	kJ/mol	Joback Method
hf	100.42	kJ/mol	Joback Method
hfus	26.34	kJ/mol	Joback Method
hvap	62.00	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	5.314		Crippen Method
mcvol	169.140	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
rinpol	1915.00		NIST Webbook
rinpol	1932.00		NIST Webbook
rinpol	1967.00		NIST Webbook
tb	654.55	K	Joback Method
tc	917.95	K	Joback Method
tf	405.16	K	Joback Method
vc	0.638	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.20	J/mol×K	654.55	Joback Method
cpg	360.92	J/mol×K	698.45	Joback Method
cpg	371.61	J/mol×K	742.35	Joback Method

cpg	381.33	J/mol×K	786.25	Joback Method
cpg	390.14	J/mol×K	830.15	Joback Method
cpg	398.13	J/mol×K	874.05	Joback Method
cpg	405.36	J/mol×K	917.95	Joback Method
dvisc	0.0010725	Pa×s	405.16	Joback Method
dvisc	0.0006985	Pa×s	446.73	Joback Method
dvisc	0.0004893	Pa×s	488.29	Joback Method
dvisc	0.0003625	Pa×s	529.86	Joback Method
dvisc	0.0002805	Pa×s	571.42	Joback Method
dvisc	0.0002248	Pa×s	612.99	Joback Method
dvisc	0.0001852	Pa×s	654.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37680696&Units=SI
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

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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume