2,3',4'-Trichloro-1,1'-biphenyl

Other names:	1,2-dichloro-4-(2-chlorophenyl)benzene
	2',3,4-Trichlorobiphenyl
	2,3',4'-Trichlorobiphenyl
	3,4,2'-Trichlorobiphenyl
	PCB 33
Inchi:	InChI=1S/C12H7Cl3/c13-10-4-2-1-3-9(10)8-5-6-11(14)12(15)7-8/h1-7H
InchiKey:	RIMXLXBUOQMDHV-UHFFFAOYSA-N
Formula:	C12H7Cl3
SMILES:	Clc1ccc(-c2ccccc2Cl)cc1Cl
Mol. weight [g/mol]:	257.55

Physical Properties

Property code	Value	Unit	Source
af	0.4532		Cheméo Relay (1.0)
gf	210.30	kJ/mol	Joback Method
hf	111.07	kJ/mol	Cheméo Relay (1.0)
hfus	26.34	kJ/mol	Joback Method
hvap	86.43	kJ/mol	Cheméo Relay (1.0)
ie	8.36	eV	Cheméo Relay (1.0)
log10ws	-6.29		Aqueous Solubility Prediction Method
logp	5.314		Crippen Method
mcvol	169.140	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
rinpol	1842.00		NIST Webbook
rinpol	1848.60		NIST Webbook
rinpol	1878.10		NIST Webbook
rinpol	1858.10		NIST Webbook
rinpol	1868.20		NIST Webbook
rinpol	1878.90		NIST Webbook
rinpol	1878.10		NIST Webbook
rinpol	1837.00		NIST Webbook
rinpol	1849.00		NIST Webbook
rinpol	1873.00		NIST Webbook
rinpol	1848.60		NIST Webbook
rinpol	1837.00		NIST Webbook
tb	599.20	K	Cheméo Relay (1.0)

tc	863.93	K	Cheméo Relay (1.0)
tf	323.94	K	Cheméo Relay (1.0)
vc	0.619	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.13	J/mol×K	874.05	Joback Method
cpg	405.36	J/mol×K	917.95	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	349.20	J/mol×K	654.55	Joback Method
dvisc	0.0004893	Pa×s	488.29	Joback Method
dvisc	0.0006985	Pa×s	446.73	Joback Method
dvisc	0.0010725	Pa×s	405.16	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
hsubt	98.20 ± 5.50	kJ/mol	320.50	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C38444869&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

Legend

af: Acentric Factor

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
hsubt:	Enthalpy of sublimation at a given temperature
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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume