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

Other names:	2,3',4-Trichloro-1,1'-biphenyl
	2,3',4-Trichlorobiphenyl
	PCB 25
Inchi:	InChI=1S/C12H7Cl3/c13-9-3-1-2-8(6-9)11-5-4-10(14)7-12(11)15/h1-7H
InchiKey:	XBBZAULFUPBZSP-UHFFFAOYSA-N
Formula:	C12H7Cl3
SMILES:	Clc1cccc(-c2ccc(Cl)cc2Cl)c1
Mol. weight [g/mol]:	257.55

Physical Properties

Property code	Value	Unit	Source
hf	109.40	kJ/mol	Cheméo Relay (1.0)
hfus	26.34	kJ/mol	Joback Method
hvap	85.14	kJ/mol	Cheméo Relay (1.0)
ie	8.36	eV	Cheméo Relay (1.0)
log10ws	-6.31		Cheméo Relay (1.0)
logp	5.314		Crippen Method
mcvol	169.140	ml/mol	McGowan Method
rinpol	1848.80		NIST Webbook
rinpol	1855.00		NIST Webbook
rinpol	1857.00		NIST Webbook
tb	596.92	K	Cheméo Relay (1.0)
tf	316.75	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	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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55712373&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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