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

Other names:	1,1'-Biphenyl, 2,2',4-trichloro- 2,2',4-Trichlorobiphenyl PCB 17
Inchi:	InChI=1S/C12H7Cl3/c13-8-5-6-10(12(15)7-8)9-3-1-2-4-11(9)14/h1-7H
InchiKey:	YKKYCYQDUUXNLN-UHFFFAOYSA-N
Formula:	C12H7Cl3
SMILES:	Clc1ccc(-c2ccccc2Cl)c(Cl)c1
Mol. weight [g/mol]:	257.54
CAS:	37680-66-3

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	1746.00		NIST Webbook
rinpol	1780.00		NIST Webbook
rinpol	1743.00		NIST Webbook
rinpol	1743.00		NIST Webbook
rinpol	1781.80		NIST Webbook
rinpol	1818.00		NIST Webbook
rinpol	1807.00		NIST Webbook
rinpol	1807.00		NIST Webbook
rinpol	1807.00		NIST Webbook
rinpol	1761.00		NIST Webbook
rinpol	1737.00		NIST Webbook
rinpol	1747.00		NIST Webbook
rinpol	1808.00		NIST Webbook
rinpol	1747.00		NIST Webbook
rinpol	1818.00		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	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
cpg	405.36	J/mol×K	917.95	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	0.0003625	Pa×s	529.86	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

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37680663&Units=SI

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

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