

2,3,3',5'-Tetrachloro-1,1'-biphenyl

Other names:	2,3,3',5'-Tetrachlorobiphenyl PCB 58
Inchi:	InChI=1S/C12H6Cl4/c13-8-4-7(5-9(14)6-8)10-2-1-3-11(15)12(10)16/h1-6H
InchiKey:	IOPBNBSKOPJKEG-UHFFFAOYSA-N
Formula:	C12H6Cl4
SMILES:	Clc1cc(Cl)cc(-c2cccc(Cl)c2Cl)c1
Mol. weight [g/mol]:	291.99

Physical Properties

Property code	Value	Unit	Source
hf	87.02	kJ/mol	Cheméo Relay (1.0)
hfus	30.15	kJ/mol	Joback Method
hvap	89.58	kJ/mol	Cheméo Relay (1.0)
ie	8.47	eV	Cheméo Relay (1.0)
log10ws	-7.07		Cheméo Relay (1.0)
logp	5.967		Crippen Method
mcvol	181.380	ml/mol	McGowan Method
rinpol	2082.00		NIST Webbook
rinpol	2082.00		NIST Webbook
rinpol	2082.00		NIST Webbook
rinpol	2084.00		NIST Webbook
tb	614.21	K	Cheméo Relay (1.0)
tf	333.72	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.27	J/mol×K	696.96	Joback Method
cpg	378.65	J/mol×K	741.36	Joback Method
cpg	388.08	J/mol×K	785.76	Joback Method
cpg	396.63	J/mol×K	830.15	Joback Method
cpg	404.36	J/mol×K	874.55	Joback Method
cpg	411.33	J/mol×K	918.95	Joback Method
cpg	417.60	J/mol×K	963.35	Joback Method

dvisc	0.0008409	Pa×s	447.60	Joback Method
dvisc	0.0005766	Pa×s	489.16	Joback Method
dvisc	0.0004195	Pa×s	530.72	Joback Method
dvisc	0.0003196	Pa×s	572.28	Joback Method
dvisc	0.0002526	Pa×s	613.84	Joback Method
dvisc	0.0002057	Pa×s	655.40	Joback Method
dvisc	0.0001717	Pa×s	696.96	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C41464497&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>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

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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