1,1'-Biphenyl, 2,3',4,6-tetrachloro-

Other names: 2,3',4,6-Tetrachlorobiphenyl
PCB 69
Inchi: InChI=1S/C12H6Cl4/c13-8-3-1-2-7(4-8)12-10(15)5-9(14)6-11(12)16/h1-6H
InchiKey: CKUBKYSLNCKBOI-UHFFFAOYSA-N
Formula: C12H6Cl4
SMILES: Clc1cccc(-c2c(Cl)cc(Cl)cc2Cl)c1
Mol. weight [g/mol]: 291.99

Physical Properties

Property code	Value	Unit	Source
hf	106.59	kJ/mol	Cheméo Relay (1.0)
hfus	30.15	kJ/mol	Joback Method
hvap	86.69	kJ/mol	Cheméo Relay (1.0)
ie	8.51	eV	Cheméo Relay (1.0)
log10ws	-6.93		Cheméo Relay (1.0)
logp	5.967		Crippen Method
mcvol	181.380	ml/mol	McGowan Method
rinpol	1890.00		NIST Webbook
rinpol	1944.00		NIST Webbook
rinpol	1893.00		NIST Webbook
rinpol	1890.00		NIST Webbook
tb	596.02	K	Cheméo Relay (1.0)
tf	338.81	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	417.60	J/mol×K	963.35	Joback Method
cpg	411.33	J/mol×K	918.95	Joback Method
cpg	404.36	J/mol×K	874.55	Joback Method
cpg	396.63	J/mol×K	830.15	Joback Method
cpg	388.08	J/mol×K	785.76	Joback Method
cpg	378.65	J/mol×K	741.36	Joback Method

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

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C60233241&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

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