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

Other names: 2,3',5'-Trichloro-1,1'-biphenyl
PCB 34
1,1'-Biphenyl, 2,3',5'-trichloro-
Inchi: InChI=1S/C12H7Cl3/c13-9-5-8(6-10(14)7-9)11-3-1-2-4-12(11)15/h1-7H
InchiKey: GXVMAQACUOSFJF-UHFFFAOYSA-N
Formula: C12H7Cl3
SMILES: Clc1cc(Cl)cc(-c2ccccc2Cl)c1
Mol. weight [g/mol]: 257.55

Physical Properties

Property code	Value	Unit	Source
af	0.4539		Cheméo Relay (1.0)
gf	210.30	kJ/mol	Joback Method
hf	114.94	kJ/mol	Cheméo Relay (1.0)
hfus	26.34	kJ/mol	Joback Method
hvap	81.84	kJ/mol	Cheméo Relay (1.0)
ie	8.46	eV	Cheméo Relay (1.0)
log10ws	-6.29		Cheméo Relay (1.0)
logp	5.314		Crippen Method
mcvol	169.140	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
rinpol	1801.00		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1814.00		NIST Webbook
rinpol	1836.00		NIST Webbook
rinpol	1836.00		NIST Webbook
rinpol	1814.00		NIST Webbook
tb	593.13	K	Cheméo Relay (1.0)
tc	848.99	K	Cheméo Relay (1.0)
tf	327.08	K	Cheméo Relay (1.0)
vc	0.615	m3/kmol	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

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=C37680685&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
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