2,4,6-Trichlorobiphenyl

Other names: 2,4,6-Trichloro-1,1'-biphenyl
PCB 30
Inchi: InChI=1S/C12H7Cl3/c13-9-6-10(14)12(11(15)7-9)8-4-2-1-3-5-8/h1-7H
InchiKey: MTLMVEWEYZFYTH-UHFFFAOYSA-N
Formula: C12H7Cl3
SMILES: Clc1cc(Cl)c(-c2ccccc2)c(Cl)c1
Mol. weight [g/mol]: 257.55

Physical Properties

Property code	Value	Unit	Source
af	0.4436		Cheméo Relay (1.0)
gf	210.30	kJ/mol	Joback Method
hf	144.02	kJ/mol	Cheméo Relay (1.0)
hfus	26.34	kJ/mol	Joback Method
hvap	77.67	kJ/mol	Cheméo Relay (1.0)
ie	8.48	eV	Cheméo Relay (1.0)
log10ws	-6.12		Aqueous Solubility Prediction Method
logp	5.314		Crippen Method
mcvol	169.140	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
rinpol	1737.00		NIST Webbook
tb	582.51	K	Cheméo Relay (1.0)
tc	851.82	K	Cheméo Relay (1.0)
tf	334.30 ± 0.20	K	NIST Webbook
vc	0.610	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	0.0006985	Pa×s	446.73	Joback Method
dvisc	0.0010725	Pa×s	405.16	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
hfust	16.50	kJ/mol	334.30	NIST Webbook
hfust	16.50	kJ/mol	334.30	NIST Webbook
hvapt	74.40	kJ/mol	368.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35693926&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

hfust: Enthalpy of fusion at a given temperature

hvap: Enthalpy of vaporization at standard conditions

hvapt: Enthalpy of vaporization at a given temperature

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