

1,1'-Biphenyl, 3,4,4'-Trichloro-

Other names:	3,4,4'-Trichlorobiphenyl PCB 37
Inchi:	InChI=1S/C12H7Cl3/c13-10-4-1-8(2-5-10)9-3-6-11(14)12(15)7-9/h1-7H
InchiKey:	YZANRISAORXTHU-UHFFFAOYSA-N
Formula:	C12H7Cl3
SMILES:	Clc1ccc(-c2ccc(Cl)c(Cl)c2)cc1
Mol. weight [g/mol]:	257.54
CAS:	38444-90-5

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	-7.06		Aqueous Solubility Prediction Method
logp	5.314		Crippen Method
mcvol	169.140	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
rinpol	1980.00		NIST Webbook
rinpol	1980.00		NIST Webbook
rinpol	2005.00		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/molxK	654.55	Joback Method
cpg	360.92	J/molxK	698.45	Joback Method
cpg	371.61	J/molxK	742.35	Joback Method

cpg	381.33	J/molxK	786.25	Joback Method
cpg	390.14	J/molxK	830.15	Joback Method
cpg	398.13	J/molxK	874.05	Joback Method
cpg	405.36	J/molxK	917.95	Joback Method
dvisc	0.0010725	Paxs	405.16	Joback Method
dvisc	0.0006985	Paxs	446.73	Joback Method
dvisc	0.0004893	Paxs	488.29	Joback Method
dvisc	0.0003625	Paxs	529.86	Joback Method
dvisc	0.0002805	Paxs	571.42	Joback Method
dvisc	0.0002248	Paxs	612.99	Joback Method
dvisc	0.0001852	Paxs	654.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38444905&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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