4-Tert-butylbiphenyl

Other names:	1,1'-biphenyl, 4-(1,1-dimethylethyl)- 4-(1,1-dimethylethyl)-1,1'-biphenyl biphenyl, 4-tert-butyl- p-tert-butylbiphenyl p-tert-butyldiphenyl
Inchi:	InChI=1S/C16H18/c1-16(2,3)15-11-9-14(10-12-15)13-7-5-4-6-8-13/h4-12H,1-3H3
InchiKey:	CDOYZTOFTGTGBC-UHFFFAOYSA-N
Formula:	C16H18
SMILES:	CC(C)(C)c1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	210.31
CAS:	1625-92-9

Physical Properties

Property code	Value	Unit	Source
gf	301.87	kJ/mol	Joback Method
hf	79.27	kJ/mol	Joback Method
hfus	19.87	kJ/mol	The heat capacities and thermodynamic functions of 4-methylbiphenyl and 4-tert-butylbiphenyl
hsub	98.10 ± 2.10	kJ/mol	NIST Webbook
hvap	80.00 ± 1.90	kJ/mol	NIST Webbook
log10ws	-5.39		Crippen Method
logp	4.651		Crippen Method
mcvol	188.780	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
tb	583.00 ± 4.00	K	NIST Webbook
tb	557.00 ± 7.00	K	NIST Webbook
tb	585.39	K	Vapour pressures and enthalpies of vaporization of a series of the alkylbiphenyls
tc	866.21	K	Joback Method
tf	324.00 ± 4.00	K	NIST Webbook
tf	325.30 ± 1.50	K	NIST Webbook
tf	325.00 ± 4.00	K	NIST Webbook
tf	325.00 ± 4.00	K	NIST Webbook
tf	324.70	K	Thermochemical studies of 4-tert-butylbiphenyl and 4,40-di-tert-butylbiphenyl

tf	325.40 ± 3.00	K	NIST Webbook
tf	325.00 ± 4.00	K	NIST Webbook
tf	325.00 ± 5.00	K	NIST Webbook
tf	330.00 ± 3.00	K	NIST Webbook
vc	0.705	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.09	J/mol×K	620.59	Joback Method
cpg	494.51	J/mol×K	661.53	Joback Method
cpg	512.38	J/mol×K	702.46	Joback Method
cpg	528.81	J/mol×K	743.40	Joback Method
cpg	543.92	J/mol×K	784.34	Joback Method
cpg	557.81	J/mol×K	825.27	Joback Method
cpg	570.60	J/mol×K	866.21	Joback Method
dvisc	0.0021349	Pa×s	337.86	Joback Method
dvisc	0.0010074	Pa×s	384.98	Joback Method
dvisc	0.0005600	Pa×s	432.10	Joback Method
dvisc	0.0003494	Pa×s	479.23	Joback Method
dvisc	0.0002372	Pa×s	526.35	Joback Method
dvisc	0.0001716	Pa×s	573.47	Joback Method
dvisc	0.0001304	Pa×s	620.59	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1625929&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapour pressures and enthalpies of vaporization of a series of the alkylbiphenyls:	https://www.doi.org/10.1016/j.fluid.2012.08.020
Thermochemical studies of 4-tert-butylbiphenyl and 4,4'-di-tert-butylbiphenyl:	https://www.doi.org/10.1016/j.jct.2008.12.015
The heat capacities and thermodynamic functions of 4-methylbiphenyl and 4-tert-butylbiphenyl :	https://www.doi.org/10.1016/j.jct.2010.05.002

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
hsub:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume