Benzene, p-di-tert-pentyl-

Other names:	1,4-bis(1,1-dimethylpropyl)benzene
	1,4-di-tert-pentylbenzene
	benzene, 1,4-bis(1,1-dimethylpropyl)-
	p-di-tert-amylbenzene
	p-di-tert-pentylbenzene
Inchi:	InChI=1S/C16H26/c1-7-15(3,4)13-9-11-14(12-10-13)16(5,6)8-2/h9-12H,7-8H2,1-6H3
InchiKey:	KNLFZJBLNQRLEL-UHFFFAOYSA-N
Formula:	C16H26
SMILES:	CCC(C)(C)c1ccc(C(C)(C)CC)cc1
Mol. weight [g/mol]:	218.38
CAS:	3373-10-2

Physical Properties

Property code	Value	Unit	Source
gf	192.30	kJ/mol	Joback Method
hf	-166.01	kJ/mol	Joback Method
hfus	16.02	kJ/mol	Joback Method
hvap	51.56	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	5.062		Crippen Method
mcvol	212.540	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
tb	533.15 ± 2.00	K	NIST Webbook
tb	545.31 ± 0.40	K	NIST Webbook
tc	803.20	K	Joback Method
tf	292.89 ± 0.20	K	NIST Webbook
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.74	J/mol×K	590.68	Joback Method
cpg	571.70	J/mol×K	626.10	Joback Method
cpg	591.30	J/mol×K	661.52	Joback Method

cpg	609.61	J/mol×K	696.94	Joback Method
cpg	626.72	J/mol×K	732.36	Joback Method
cpg	642.72	J/mol×K	767.78	Joback Method
cpg	657.69	J/mol×K	803.20	Joback Method
dvisc	0.0035793	Pa×s	313.86	Joback Method
dvisc	0.0014107	Pa×s	360.00	Joback Method
dvisc	0.0006870	Pa×s	406.13	Joback Method
dvisc	0.0003874	Pa×s	452.27	Joback Method
dvisc	0.0002429	Pa×s	498.41	Joback Method
dvisc	0.0001649	Pa×s	544.54	Joback Method
dvisc	0.0001189	Pa×s	590.68	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemistry of ionic liquid-catalysed reactions. Isomerisation and transalkylation of tert-alkyl-benzenes. Are these systems ideal?:	https://www.doi.org/10.1016/j.jct.2010.01.006
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=C3373102&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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