

1,4-Ditertiary butylbenzene

Other names:	1,4-bis(1,1-dimethylethyl)benzene 1,4-di-tert-butylbenzene Benzene, 1,4-bis-(tert-butyl) Benzene, p-di-tert-butyl- benzene, 1,4-di-tert-butyl- p-di-tert-butylbenzene
Inchi:	InChI=1S/C14H22/c1-13(2,3)11-7-9-12(10-8-11)14(4,5)6/h7-10H,1-6H3
InchiKey:	OOWNNCMFKFBNOF-UHFFFAOYSA-N
Formula:	C14H22
SMILES:	CC(C)(C)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]:	190.33
CAS:	1012-72-2

Physical Properties

Property code	Value	Unit	Source
af	0.3997		Cheméo Relay (1.0)
hf	-120.40	kJ/mol	Cheméo Relay (1.0)
hfl	-188.90 ± 1.50	kJ/mol	NIST Webbook
hfus	8.21	kJ/mol	Thermodynamic properties of tert-butylbenzene and 1,4-di-tert-butylbenzene
hsub	82.80 ± 0.40	kJ/mol	
hsub	82.80 ± 0.40	kJ/mol	NIST Webbook
hvap	63.00 ± 0.10	kJ/mol	NIST Webbook
hvap	63.00 ± 0.60	kJ/mol	NIST Webbook
hvap	61.40 ± 0.30	kJ/mol	NIST Webbook
ie	8.11	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.28	eV	NIST Webbook
ie	8.24 ± 0.02	eV	NIST Webbook
ie	8.31	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
ie	8.74 ± 0.07	eV	NIST Webbook
log10ws	-6.02		Cheméo Relay (1.0)
logp	4.282		Crippen Method
mcvol	184.360	ml/mol	McGowan Method
pc	2300.00 ± 200.00	kPa	NIST Webbook
rhoc	260.74 ± 15.04	kg/m3	NIST Webbook

rinpol	1281.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1319.00		NIST Webbook
rinpol	1314.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1281.00		NIST Webbook
ripol	1495.10		NIST Webbook
ripol	1504.00		NIST Webbook
ripol	1488.00		NIST Webbook
ripol	1488.00		NIST Webbook
ripol	1552.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1528.00		NIST Webbook
ripol	1516.00		NIST Webbook
ripol	1515.00		NIST Webbook
tb	508.15 ± 2.00	K	NIST Webbook
tc	708.00 ± 2.00	K	NIST Webbook
tf	351.00 ± 2.00	K	NIST Webbook
tf	349.15 ± 1.50	K	NIST Webbook
tf	360.40 ± 1.50	K	NIST Webbook
tf	351.40 ± 2.00	K	NIST Webbook
tf	350.76 ± 0.01	K	NIST Webbook
tf	349.80 ± 0.30	K	NIST Webbook
tf	348.00 ± 4.00	K	NIST Webbook
tf	349.90 ± 1.00	K	NIST Webbook
tf	349.90 ± 0.70	K	NIST Webbook
tf	350.40 ± 0.30	K	NIST Webbook
tt	350.80 ± 0.30	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.95	J/mol×K	764.89	Joback Method
cpg	521.50	J/mol×K	691.57	Joback Method
cpg	505.11	J/mol×K	654.91	Joback Method
cpg	536.75	J/mol×K	728.23	Joback Method
cpg	448.22	J/mol×K	544.92	Joback Method
cpg	468.56	J/mol×K	581.58	Joback Method
cpg	487.49	J/mol×K	618.24	Joback Method
dvisc	0.0042689	Pa×s	291.32	Joback Method
dvisc	0.0002085	Pa×s	502.65	Joback Method

dvisc	0.0008490	Pa×s	375.85	Joback Method
dvisc	0.0017186	Pa×s	333.59	Joback Method
dvisc	0.0003055	Pa×s	460.39	Joback Method
dvisc	0.0004837	Pa×s	418.12	Joback Method
dvisc	0.0001510	Pa×s	544.92	Joback Method
hfust	22.48	kJ/mol	341.50	NIST Webbook
hfust	8.20	kJ/mol	350.80	NIST Webbook
hsubt	82.10 ± 0.40	kJ/mol	310.50	NIST Webbook
hsubt	82.80	kJ/mol	305.00	NIST Webbook
hvapt	55.80 ± 0.10	kJ/mol	439.00	NIST Webbook
hvapt	44.60 ± 0.30	kJ/mol	439.00	NIST Webbook
hvapt	46.40 ± 0.20	kJ/mol	439.00	NIST Webbook
hvapt	61.40 ± 0.10	kJ/mol	439.00	NIST Webbook
hvapt	54.60 ± 0.10	kJ/mol	439.00	NIST Webbook
pvap	0.38	kPa	354.15	Study and prediction of alkylbenzenes vapour pressures
pvap	0.72	kPa	366.55	Study and prediction of alkylbenzenes vapour pressures
pvap	0.81	kPa	369.15	Study and prediction of alkylbenzenes vapour pressures
pvap	0.94	kPa	372.05	Study and prediction of alkylbenzenes vapour pressures
pvap	1.04	kPa	374.15	Study and prediction of alkylbenzenes vapour pressures
pvap	1.17	kPa	376.45	Study and prediction of alkylbenzenes vapour pressures
pvap	1.38	kPa	379.75	Study and prediction of alkylbenzenes vapour pressures
pvap	1.51	kPa	381.75	Study and prediction of alkylbenzenes vapour pressures
pvap	1.65	kPa	383.25	Study and prediction of alkylbenzenes vapour pressures
pvap	0.72	kPa	366.45	Study and prediction of alkylbenzenes vapour pressures

pvap	0.65	kPa	364.25	Study and prediction of alkylbenzenes vapour pressures
pvap	0.57	kPa	361.75	Study and prediction of alkylbenzenes vapour pressures
pvap	0.49	kPa	358.95	Study and prediction of alkylbenzenes vapour pressures
pvap	0.43	kPa	356.45	Study and prediction of alkylbenzenes vapour pressures

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49987e+01
Coeff. B	-4.41062e+03
Coeff. C	-8.32500e+01
Temperature range (K), min.	383.07
Temperature range (K), max.	538.55

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1012722&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Thermodynamic properties of tert-butylbenzene and New data on the relationship between the enthalpies of fusion of aromatic compounds and the melting temperatures and the enthalpies of solution in benzene at 298.15 K. Part I: McGowan Method.	https://www.doi.org/10.1016/j.jct.2008.10.008 https://www.doi.org/10.1016/j.jct.2017.09.006 https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure http://link.springer.com/article/10.1007/BF02311772
Study and prediction of alkylbenzenes vapour pressures: Crippen Method:	https://www.doi.org/10.1016/j.fluid.2008.04.016 https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Thermochemistry of ionic liquid-catalysed reactions. Isomerisation and transalkylation of tert-alkyl-benzenes. Are these systems ideal?: Cheméo Relay (1.0 beta)	https://www.doi.org/10.1016/j.jct.2010.01.006

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation 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
pvap:	Vapor pressure
rhoc:	Critical density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

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