

Benzene, 1,4-bis(1,1-dimethylethyl)-

Other names:	1,4-Di-tert-butylbenzene 1,4-bis(1,1-dimethylethyl)benzene 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]:	190.32
CAS:	1012-72-2

Physical Properties

Property code	Value	Unit	Source
gf	175.46	kJ/mol	Joback Method
hf	-124.73	kJ/mol	Joback Method
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 ± 0.60	kJ/mol	NIST Webbook
hvap	61.40 ± 0.30	kJ/mol	NIST Webbook
hvap	63.00 ± 0.10	kJ/mol	NIST Webbook
ie	8.74 ± 0.07	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
ie	8.11	eV	NIST Webbook
ie	8.31	eV	NIST Webbook
ie	8.28	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.24 ± 0.02	eV	NIST Webbook
log10ws	-4.10		Crippen Method
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	1281.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1319.00		NIST Webbook
rinpol	1314.00		NIST Webbook
rinpol	1298.00		NIST Webbook
ripol	1495.10		NIST Webbook
ripol	1515.00		NIST Webbook
ripol	1516.00		NIST Webbook
ripol	1528.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1552.00		NIST Webbook
ripol	1504.00		NIST Webbook
ripol	1488.00		NIST Webbook
ripol	1488.00		NIST Webbook
tb	508.15 ± 2.00	K	NIST Webbook
tc	708.00 ± 2.00	K	NIST Webbook
tf	291.32	K	Joback Method
tt	350.80 ± 0.30	K	NIST Webbook
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	505.11	J/mol×K	654.91	Joback Method
cpg	521.50	J/mol×K	691.57	Joback Method
cpg	536.75	J/mol×K	728.23	Joback Method
cpg	550.95	J/mol×K	764.89	Joback Method
dvisc	0.0008490	Pa×s	375.85	Joback Method
dvisc	0.0017186	Pa×s	333.59	Joback Method
dvisc	0.0042689	Pa×s	291.32	Joback Method
dvisc	0.0004837	Pa×s	418.12	Joback Method
dvisc	0.0003055	Pa×s	460.39	Joback Method
dvisc	0.0002085	Pa×s	502.65	Joback Method
dvisc	0.0001510	Pa×s	544.92	Joback Method
hfust	8.20	kJ/mol	350.80	NIST Webbook
hfust	22.48	kJ/mol	341.50	NIST Webbook
hsubt	82.10 ± 0.40	kJ/mol	310.50	NIST Webbook

hsubt	82.80	kJ/mol	305.00	NIST Webbook	
hvapt	44.60 ± 0.30	kJ/mol	439.00	NIST Webbook	
hvapt	54.60 ± 0.10	kJ/mol	439.00	NIST Webbook	
hvapt	61.40 ± 0.10	kJ/mol	439.00	NIST Webbook	
hvapt	46.40 ± 0.20	kJ/mol	439.00	NIST Webbook	
hvapt	55.80 ± 0.10	kJ/mol	439.00	NIST Webbook	
pvap	0.38	kPa	354.15	Study and prediction of alkylbenzenes vapour pressures	
pvap	0.43	kPa	356.45	Study and prediction of alkylbenzenes vapour pressures	
pvap	0.49	kPa	358.95	Study and prediction of alkylbenzenes vapour pressures	
pvap	0.57	kPa	361.75	Study and prediction of alkylbenzenes vapour pressures	
pvap	0.65	kPa	364.25	Study and prediction of alkylbenzenes vapour pressures	
pvap	0.72	kPa	366.45	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

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

Thermodynamic properties of tert-butylbenzene and isobutylbenzene:	https://www.doi.org/10.1016/j.jct.2008.10.008
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Study and prediction of alkylbenzenes vapour pressures:	https://www.doi.org/10.1016/j.fluid.2008.04.016
Thermochemistry of ionic liquid-catalysed reactions.	https://www.doi.org/10.1016/j.jct.2010.01.006
The Yaws Handbook of Vapor Pressure and Transylation of Organic Compounds	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Isomerisation and transylation of alkylbenzenes. Are these systems ideal?	http://link.springer.com/article/10.1007/BF02311772
McCowan Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1012722&Units=SI
NIST Webbook:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Crippen Method:	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation

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
vc:	Critical Volume

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