Benzene, 1,3-bis(1,1-dimethylethyl)-

Other names:	1,3-Di-tert-butylbenzene
	1,3-Ditertiarybutylbenzene
	1,3-bis(1,1-Dimethylethyl)benzene
	Benzene, m-di-tert-butyl-
	m-Di-tert-butylbenzene
Inchi:	InChI=1S/C14H22/c1-13(2,3)11-8-7-9-12(10-11)14(4,5)6/h7-10H,1-6H3
InchiKey:	ILNDSSCEZZFNGE-UHFFFAOYSA-N
Formula:	C14H22
SMILES:	CC(C)(C)c1cccc(C(C)(C)C)c1
Mol. weight [g/mol]:	190.32
CAS:	1014-60-4

Physical Properties

Property code	Value	Unit	Source
gf	175.46	kJ/mol	Joback Method
hf	-124.73	kJ/mol	Joback Method
hfl	-187.40 ± 1.50	kJ/mol	NIST Webbook
hfus	10.84	kJ/mol	Joback Method
hvap	59.60 ± 0.50	kJ/mol	NIST Webbook
ie	8.71 ± 0.07	eV	NIST Webbook
ie	8.43	eV	NIST Webbook
log10ws	-4.10		Crippen Method
logp	4.282		Crippen Method
mcvol	184.360	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
rinpol	1249.00		NIST Webbook
rinpol	1245.00		NIST Webbook
ripol	1454.00		NIST Webbook
ripol	1420.00		NIST Webbook
ripol	1444.00		NIST Webbook
ripol	1436.00		NIST Webbook
ripol	1427.00		NIST Webbook
ripol	1426.00		NIST Webbook
tb	544.92	K	Joback Method
tc	764.89	K	Joback Method
tf	291.32	K	Joback Method
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	0.0017186	Pa×s	333.59	Joback Method
dvisc	0.0042689	Pa×s	291.32	Joback Method
dvisc	0.0008490	Pa×s	375.85	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
hvapt	58.90 ± 0.50	kJ/mol	310.50	NIST Webbook
hvapt	58.00	kJ/mol	360.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	379.70	K	2.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38447e+01
Coeff. B	-4.12602e+03
Coeff. C	-8.68040e+01
Temperature range (K), min.	391.15

Temperature range (K), max.	570.33

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C1014604&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume