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

Other names:	1,4-BIS(1-METHYLETHYL)BENZENE
	1,4-DIISOPROPYLBENZENE
	4-Isopropylcumene
	Benzene, 1,4-di-(1-methylethyl)
	Benzene, 1,4-diisopropyl-
	Benzene, p-diisopropyl-
	p-Diisopropylbenzene
	p-bis(1-methylethyl)benzene
Inchi:	InChI=1S/C12H18/c1-9(2)11-5-7-12(8-6-11)10(3)4/h5-10H,1-4H3
InchiKey:	SPPWGCYEYAMHDT-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	CC(C)c1ccc(C(C)C)cc1
Mol. weight [g/mol]:	162.27
CAS:	100-18-5

Physical Properties

Property code	Value	Unit	Source
gf	148.06	kJ/mol	Joback Method
hf	-76.51	kJ/mol	Joback Method
hfl	-132.30	kJ/mol	NIST Webbook
hfus	13.44	kJ/mol	Joback Method
hvap	56.50 ± 0.30	kJ/mol	NIST Webbook
ie	8.35	eV	NIST Webbook
log10ws	-3.84		Crippen Method
logp	3.933		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	9777.86 ± 405.30	kPa	NIST Webbook
pc	2360.00	kPa	Critical Point and Vapor Pressure Measurements for 17 Compounds by a Low Residence Time Flow Method
pc	2358.00	kPa	KDB
rinpol	1152.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1143.00		NIST Webbook

rinpol	1157.00	NIST Webbook
rinpol	1162.00	NIST Webbook
rinpol	1168.00	NIST Webbook
rinpol	1162.00	NIST Webbook
rinpol	1161.00	NIST Webbook
rinpol	1158.00	NIST Webbook
rinpol	1160.00	NIST Webbook
rinpol	1158.00	NIST Webbook
rinpol	1174.70	NIST Webbook
rinpol	1173.40	NIST Webbook
rinpol	1170.10	NIST Webbook
rinpol	1160.90	NIST Webbook
rinpol	1154.40	NIST Webbook
rinpol	1174.70	NIST Webbook
rinpol	1160.00	NIST Webbook
rinpol	1173.40	NIST Webbook
rinpol	1170.10	NIST Webbook
rinpol	1183.00	NIST Webbook
rinpol	1159.50	NIST Webbook
rinpol	1179.00	NIST Webbook
rinpol	1152.70	NIST Webbook
rinpol	1152.10	NIST Webbook
rinpol	1168.70	NIST Webbook
rinpol	1168.90	NIST Webbook
rinpol	1151.20	NIST Webbook
rinpol	1160.00	NIST Webbook
rinpol	1162.00	NIST Webbook
rinpol	1167.00	NIST Webbook
rinpol	1171.00	NIST Webbook
rinpol	1151.20	NIST Webbook
rinpol	1153.40	NIST Webbook
rinpol	1161.60	NIST Webbook
rinpol	1166.70	NIST Webbook
rinpol	1171.30	NIST Webbook
rinpol	1158.00	NIST Webbook
rinpol	1153.40	NIST Webbook
rinpol	1154.00	NIST Webbook
rinpol	1148.55	NIST Webbook
rinpol	1162.00	NIST Webbook
ripol	1380.70	NIST Webbook
ripol	1426.00	NIST Webbook
ripol	1418.00	NIST Webbook
ripol	1358.00	NIST Webbook
ripol	1392.00	NIST Webbook

ripol	1435.00		NIST Webbook
ripol	1412.00		NIST Webbook
ripol	1402.00		NIST Webbook
ripol	1402.00		NIST Webbook
ripol	1404.00		NIST Webbook
ripol	1417.60		NIST Webbook
tb	477.65 ± 1.50	K	NIST Webbook
tb	483.50	K	NIST Webbook
tb	483.45	K	KDB
tb	483.50 ± 2.00	K	NIST Webbook
tb	477.00 ± 8.00	K	NIST Webbook
tb	483.52 ± 2.00	K	NIST Webbook
tc	794.15 ± 3.00	K	NIST Webbook
tc	674.75	K	KDB
tf	256.11 ± 0.02	K	NIST Webbook
tf	256.05	K	KDB
tf	256.08 ± 1.00	K	NIST Webbook
tf	256.12 ± 0.01	K	NIST Webbook
tf	256.11 ± 0.02	K	NIST Webbook
tf	256.07 ± 0.05	K	NIST Webbook
vc	0.584	m3/kmol	KDB
zc	0.2455420		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.55	J/mol×K	714.27	Joback Method
cpg	346.60	J/mol×K	504.74	Joback Method
cpg	364.01	J/mol×K	539.66	Joback Method
cpg	380.47	J/mol×K	574.58	Joback Method
cpg	396.02	J/mol×K	609.51	Joback Method
cpg	410.70	J/mol×K	644.43	Joback Method
cpg	424.53	J/mol×K	679.35	Joback Method
dvisc	0.0001786	Pa×s	504.74	Joback Method
dvisc	0.0055461	Pa×s	233.94	Joback Method
dvisc	0.0019687	Pa×s	279.07	Joback Method
dvisc	0.0009324	Pa×s	324.21	Joback Method
dvisc	0.0005301	Pa×s	369.34	Joback Method
dvisc	0.0003408	Pa×s	414.47	Joback Method
dvisc	0.0002390	Pa×s	459.61	Joback Method
hvapt	48.90	kJ/mol	439.00	NIST Webbook

hvapt	50.70 ± 0.20	kJ/mol	448.00	NIST Webbook
hvapt	46.30 ± 0.30	kJ/mol	448.00	NIST Webbook
hvapt	43.00 ± 0.50	kJ/mol	448.00	NIST Webbook
hvapt	39.30 ± 0.90	kJ/mol	448.00	NIST Webbook
hvapt	56.30 ± 0.30	kJ/mol	300.50	NIST Webbook
hvapt	47.60	kJ/mol	439.00	NIST Webbook
rhol	860.05	kg/m3	293.10	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.34508e+01
Coeff. B	-3.72488e+03
Coeff. C	-7.54240e+01
Temperature range (K), min.	358.40
Temperature range (K), max.	533.06

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.62940e+01
Coeff. B	-9.69497e+03
Coeff. C	-1.00850e+01
Coeff. D	3.10925e-06
Temperature range (K), min.	256.08
Temperature range (K), max.	689.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=701
Critical Point and Vapor Pressure Measurements for 17 Compounds by a Low Residence Time Flow Method:	https://www.doi.org/10.1021/je060269j
KDB:	https://www.cheric.org/files/research/kdb/mol/mol701.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100185&Units=SI

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility