Benzene, hexamethyl-

Other names:	1,2,3,4,5,6-Hexamethylbenzene
	HEXAMETHYLBENZENE
	MELLITENE
Inchi:	InChI=1S/C12H18/c1-7-8(2)10(4)12(6)11(5)9(7)3/h1-6H3
InchiKey:	YUWFEBAXEOLKSG-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	Cc1c(C)c(C)c(C)c(C)c1C
Mol. weight [g/mol]:	162.27
CAS:	87-85-4

Physical Properties

Property code	Value	Unit	Source
af	0.3960		KDB
affp	860.60	kJ/mol	NIST Webbook
basg	836.00	kJ/mol	NIST Webbook
chl	-7134.60 ± 7.10	kJ/mol	NIST Webbook
chs	-7132.20 ± 1.90	kJ/mol	NIST Webbook
chs	-7131.30 ± 3.00	kJ/mol	NIST Webbook
chs	-7113.20 ± 5.20	kJ/mol	NIST Webbook
ea	0.12 ± 0.02	eV	NIST Webbook
gf	114.42	kJ/mol	Joback Method
hf	-78.30	kJ/mol	NIST Webbook
hf	-77.40 ± 2.50	kJ/mol	NIST Webbook
hfl	-142.00	kJ/mol	NIST Webbook
hfs	-163.30 ± 3.10	kJ/mol	NIST Webbook
hfs	-162.40 ± 2.50	kJ/mol	NIST Webbook
hfus	18.93	kJ/mol	Joback Method
hsub	86.10	kJ/mol	NIST Webbook
hsub	81.41 ± 0.11	kJ/mol	NIST Webbook
hsub	81.40 ± 0.10	kJ/mol	NIST Webbook
hsub	85.00 ± 0.20	kJ/mol	NIST Webbook
hsub	85.00	kJ/mol	NIST Webbook
hsub	85.00 ± 0.20	kJ/mol	NIST Webbook
hsub	74.89 ± 0.63	kJ/mol	NIST Webbook
hvap	68.60	kJ/mol	NIST Webbook
ie	7.85	eV	NIST Webbook
ie	7.85 ± 0.01	eV	NIST Webbook

ie	7.85	eV	NIST Webbook
ie	7.85 ± 0.02	eV	NIST Webbook
ie	7.87	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
ie	7.95	eV	NIST Webbook
ie	7.85	eV	NIST Webbook
ie	7.90	eV	NIST Webbook
log10ws	-5.23		Aqueous Solubility Prediction Method
log10ws	-5.23		Estimated Solubility Method
logp	3.537		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2240.00	kPa	KDB
rinpol	1437.00		NIST Webbook
rinpol	1437.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1441.60		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1415.60		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1452.40		NIST Webbook
rinpol	1416.00		NIST Webbook
rinpol	1428.20		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1431.00		NIST Webbook
ripol	1778.00		NIST Webbook
ripol	1778.00		NIST Webbook
ss	309.60	J/mol×K	NIST Webbook
ss	302.81	J/mol×K	NIST Webbook
ss	306.31	J/mol×K	NIST Webbook
tb	536.60	K	KDB
tb	538.20	K	NIST Webbook
tb	536.85 ± 0.60	K	NIST Webbook
tc	758.00 ± 2.00	K	NIST Webbook
tc	751.15 ± 10.00	K	NIST Webbook
tc	758.00 ± 1.00	K	NIST Webbook
tc	758.00	K	KDB
tf	439.60	K	KDB
tf	438.55	K	Aqueous Solubility Prediction Method
vc	0.600	m3/kmol	KDB
zc	0.2130740		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.53	J/mol×K	730.53	Joback Method
cpg	404.77	J/mol×K	662.20	Joback Method
cpg	391.48	J/mol×K	628.03	Joback Method
cpg	377.58	J/mol×K	593.87	Joback Method
cpg	363.06	J/mol×K	559.70	Joback Method
cpg	347.90	J/mol×K	525.54	Joback Method
cpg	417.45	J/mol×K	696.36	Joback Method
cpl	370.70	J/mol×K	455.00	NIST Webbook
cps	254.80	J/mol×K	294.60	NIST Webbook
cps	258.50	J/mol×K	303.00	NIST Webbook
cps	256.10	J/mol×K	293.81	NIST Webbook
cps	245.64	J/mol×K	298.15	NIST Webbook
cps	252.11	J/mol×K	300.00	NIST Webbook
cps	243.40	J/mol×K	298.15	NIST Webbook
dvisc	0.0001772	Pa×s	525.54	Joback Method
dvisc	0.0003177	Pa×s	419.78	Joback Method
dvisc	0.0002538	Pa×s	455.03	Joback Method
dvisc	0.0008438	Pa×s	314.02	Joback Method
dvisc	0.0005705	Pa×s	349.27	Joback Method
dvisc	0.0004145	Pa×s	384.53	Joback Method
dvisc	0.0002094	Pa×s	490.29	Joback Method
hfust	20.63	kJ/mol	438.70	NIST Webbook
hfust	1.76	kJ/mol	383.70	NIST Webbook
hfust	20.63	kJ/mol	438.70	NIST Webbook
hsubt	83.20	kJ/mol	339.00	NIST Webbook
hsubt	85.20	kJ/mol	320.50	NIST Webbook
hvapt	56.80	kJ/mol	490.00	NIST Webbook
hvapt	68.56	kJ/mol	298.00	Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons. Liquid-Vapor Pressure Isotope Effects
sfust	4.58	J/mol×K	383.70	NIST Webbook
sfust	47.02	J/mol×K	438.70	NIST Webbook
srf	0.02	N/m	453.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45324e+01
Coeff. B	-4.38305e+03
Coeff. C	-9.44990e+01
Temperature range (K), min.	402.19
Temperature range (K), max.	569.83

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.32512e+02
Coeff. B	-2.47005e+04
Coeff. C	-4.56974e+01
Coeff. D	1.87990e-05
Temperature range (K), min.	302.15
Temperature range (K), max.	758.00

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=705

Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons: https://www.doi.org/10.1021/je800091s

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C87854&Units=SI

Liquid-Vapor Pressure Isotope Effects: http://

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=705

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfs:	Solid 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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
srf:	Surface Tension
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility