Benzene, pentamethyl-

Other names:	1,2,3,4,5-PENTAMETHYLBENZENE Benzene, 1,2,3,4,5-pentamethyl- Pentamethylbenzene
Inchi:	InChI=1S/C11H16/c1-7-6-8(2)10(4)11(5)9(7)3/h6H,1-5H3
InchiKey:	BEZDDPMMPIDMGJ-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	Cc1cc(C)c(C)c(C)c1C
Mol. weight [g/mol]:	148.24
CAS:	700-12-9

Physical Properties

Property code	Value	Unit	Source
af	0.4070		KDB
affp	850.70	kJ/mol	NIST Webbook
basg	823.50	kJ/mol	NIST Webbook
chl	-6475.60 ± 6.30	kJ/mol	NIST Webbook
chs	-6470.60 ± 1.60	kJ/mol	NIST Webbook
chs	-6480.10 ± 2.60	kJ/mol	NIST Webbook
ea	0.18 ± 0.01	eV	NIST Webbook
gf	115.63	kJ/mol	Joback Method
hf	-67.20 ± 2.20	kJ/mol	NIST Webbook
hf	-57.70	kJ/mol	NIST Webbook
hfs	-144.60 ± 2.20	kJ/mol	NIST Webbook
hfs	-135.10 ± 2.60	kJ/mol	NIST Webbook
hfus	16.73	kJ/mol	Joback Method
hsub	77.40 ± 0.40	kJ/mol	NIST Webbook
hsub	71.60 ± 0.10	kJ/mol	NIST Webbook
hsub	71.60 ± 0.10	kJ/mol	NIST Webbook
hsub	77.40 ± 0.40	kJ/mol	NIST Webbook
hsub	77.40	kJ/mol	NIST Webbook
hvap	45.00	kJ/mol	Joback Method
ie	7.92 ± 0.02	eV	NIST Webbook
ie	7.92	eV	NIST Webbook
ie	7.92	eV	NIST Webbook
ie	7.92	eV	NIST Webbook
ie	7.90	eV	NIST Webbook

log10ws	-4.00		Aqueous Solubility Prediction Method
log10ws	-4.00		Estimated Solubility Method
logp	3.229		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2490.00	kPa	KDB
rinpol	1253.90		NIST Webbook
rinpol	1258.60		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1274.15		NIST Webbook
rinpol	1265.42		NIST Webbook
rinpol	1265.49		NIST Webbook
rinpol	1265.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1290.40		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	218.10		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1281.80		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1270.40		NIST Webbook
rinpol	1251.20		NIST Webbook
rinpol	1265.42		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1253.90		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1292.60		NIST Webbook
rinpol	1281.80		NIST Webbook
rinpol	1280.50		NIST Webbook
rinpol	1270.40		NIST Webbook
rinpol	1260.30		NIST Webbook
rinpol	1258.60		NIST Webbook
rinpol	1251.20		NIST Webbook
rinpol	1268.00		NIST Webbook
rinpol	1260.00		NIST Webbook
ripol	1666.70		NIST Webbook

ripol	1644.50		NIST Webbook
ripol	1644.50		NIST Webbook
ss	294.10	J/mol×K	NIST Webbook
tb	503.40 ± 1.50	K	NIST Webbook
tb	503.15 ± 2.00	K	NIST Webbook
tb	504.00 ± 2.00	K	NIST Webbook
tb	503.00 ± 3.00	K	NIST Webbook
tb	540.00 ± 6.00	K	NIST Webbook
tb	505.15 ± 0.60	K	NIST Webbook
tb	503.00 ± 3.00	K	NIST Webbook
tb	505.20	K	NIST Webbook
tb	505.10	K	KDB
tb	486.00 ± 6.00	K	NIST Webbook
tb	503.00 ± 3.00	K	NIST Webbook
tc	719.00	K	KDB
tf	327.40	K	Aqueous Solubility Prediction Method
tf	327.50	K	KDB
vc	0.543	m3/kmol	KDB
zc	0.2263780		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.10	J/mol×K	601.11	Joback Method
cpg	380.26	J/mol×K	704.55	Joback Method
cpg	368.79	J/mol×K	670.07	Joback Method
cpg	356.74	J/mol×K	635.59	Joback Method
cpg	330.85	J/mol×K	566.64	Joback Method
cpg	302.47	J/mol×K	497.68	Joback Method
cpg	316.97	J/mol×K	532.16	Joback Method
cps	270.30	J/mol×K	298.10	NIST Webbook
cps	267.30	J/mol×K	303.00	NIST Webbook
cps	251.00	J/mol×K	283.80	NIST Webbook
cps	210.50	J/mol×K	298.15	NIST Webbook
dvisc	0.0002749	Pa×s	428.53	Joback Method
dvisc	0.0010148	Pa×s	290.23	Joback Method
dvisc	0.0006596	Pa×s	324.81	Joback Method
dvisc	0.0004658	Pa×s	359.38	Joback Method
dvisc	0.0001878	Pa×s	497.68	Joback Method
dvisc	0.0002240	Pa×s	463.11	Joback Method

dvisc	0.0003496	Pa×s	393.96	Joback Method
hfust	10.67	kJ/mol	328.20	NIST Webbook
hfust	1.98	kJ/mol	296.80	NIST Webbook
hfust	10.67	kJ/mol	328.20	NIST Webbook
hfust	10.67	kJ/mol	328.20	NIST Webbook
hvapt	57.80	kJ/mol	420.50	NIST Webbook
sfust	32.50	J/mol×K	328.20	NIST Webbook
sfust	6.67	J/mol×K	296.80	NIST Webbook
sfust	32.51	J/mol×K	328.20	NIST Webbook
srf	0.02	N/m	373.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43421e+01
Coeff. B	-4.14581e+03
Coeff. C	-7.81920e+01
Temperature range (K), min.	373.17
Temperature range (K), max.	537.28

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.61243e+02
Coeff. B	-1.35972e+04
Coeff. C	-2.13080e+01
Coeff. D	1.14973e-05
Temperature range (K), min.	338.15
Temperature range (K), max.	543.00

Sources

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

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=697
KDB:	https://www.cheric.org/files/research/kdb/mol/mol697.mol
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C700129&Units=SI

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
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
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
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