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

Other names:	1,3-DIISOPROPYLBENZENE
	1,3-bis(1-methylethyl)benzene
	3-Isopropylcumene
	Benzene, 1,3-di-(1-methylethyl)
	Benzene, m-diisopropyl-
	m-Diisopropylbenzene
	meta-Diisopropylbenzene
Inchi:	InChI=1S/C12H18/c1-9(2)11-6-5-7-12(8-11)10(3)4/h5-10H,1-4H3
InchiKey:	UNEATYXSUBPPKP-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	CC(C)c1cccc(C(C)C)c1
Mol. weight [g/mol]:	162.27
CAS:	99-62-7

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	56.20 ± 0.80	kJ/mol	NIST Webbook
log10ws	-3.84		Crippen Method
logp	3.933		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2349.00	kPa	KDB
rinpol	1141.00		NIST Webbook
rinpol	1116.70		NIST Webbook
rinpol	1122.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1113.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1141.00		NIST Webbook

rinpol	1136.20		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1142.75		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1135.20		NIST Webbook
rinpol	1115.13		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1146.80		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1116.30		NIST Webbook
rinpol	1118.80		NIST Webbook
rinpol	1142.70		NIST Webbook
rinpol	1118.80		NIST Webbook
rinpol	1150.70		NIST Webbook
rinpol	1122.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1376.00		NIST Webbook
ripol	1331.00		NIST Webbook
ripol	1321.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1389.00		NIST Webbook
ripol	1380.00		NIST Webbook
ripol	1370.00		NIST Webbook
ripol	1362.00		NIST Webbook
ripol	1362.00		NIST Webbook
ripol	1361.00		NIST Webbook
ripol	1376.00		NIST Webbook
ripol	1354.00		NIST Webbook
ripol	1342.20		NIST Webbook
tb	476.40	K	NIST Webbook
tb	476.35	K	KDB
tb	476.20 ± 2.00	K	NIST Webbook
tb	476.33 ± 2.00	K	NIST Webbook
tc	664.35	K	KDB
tf	210.02 ± 2.00	K	NIST Webbook
tf	210.05	K	KDB

vc	0.583	m3/kmol	KDB
zc	0.2478810		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	437.55	J/mol×K	714.27	Joback Method
dvisc	0.0019687	Pa×s	279.07	Joback Method
dvisc	0.0055461	Pa×s	233.94	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
dvisc	0.0001786	Pa×s	504.74	Joback Method
hvapt	56.00 ± 0.80	kJ/mol	300.50	NIST Webbook
hvapt	48.90	kJ/mol	432.00	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	1.41482e+01
Coeff. B	-3.94159e+03
Coeff. C	-6.27270e+01
Temperature range (K), min.	347.10
Temperature range (K), max.	508.77

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.11326e+01
Coeff. B	-8.76552e+03
Coeff. C	-7.87128e+00
Coeff. D	1.85746e-06
Temperature range (K), min.	210.02
Temperature range (K), max.	684.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol700.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99627&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=700

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
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