Benzene, 1-ethyl-2,3-dimethyl-

Other names:	1,2-DIMETHYL-3-ETHYLBENZENE
	1-Ethyl-2,3-dimethylbenzene
	3-Ethyl-1,2-dimethylbenzene
	3-Ethyl-o-xylene
	o-Xylene, 3-ethyl-
Inchi:	InChI=1S/C10H14/c1-4-10-7-5-6-8(2)9(10)3/h5-7H,4H2,1-3H3
InchiKey:	QUBBAXISAHIDNM-UHFFFAOYSA-N
Formula:	C10H14
SMILES:	CCc1cccc(C)c1C
Mol. weight [g/mol]:	134.22
CAS:	933-98-2

Physical Properties

Property code	Value	Unit	Source
af	0.4070		KDB
chl	-5853.00 ± 2.60	kJ/mol	NIST Webbook
chl	-5855.40 ± 1.20	kJ/mol	NIST Webbook
gf	126.47	kJ/mol	Joback Method
hf	-36.14	kJ/mol	Joback Method
hfl	-83.00 ± 2.60	kJ/mol	NIST Webbook
hfl	-80.50 ± 1.30	kJ/mol	NIST Webbook
hfus	14.92	kJ/mol	Joback Method
hvap	54.90	kJ/mol	NIST Webbook
log10ws	-3.23		Crippen Method
logp	2.866		Crippen Method
mcvol	128.000	ml/mol	McGowan Method
pc	2929.00	kPa	KDB
rinpol	1094.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1096.50		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1088.00		NIST Webbook

rinpol	1085.00	NIST Webbook
rinpol	1113.10	NIST Webbook
rinpol	1088.00	NIST Webbook
rinpol	1087.00	NIST Webbook
rinpol	1095.40	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1101.00	NIST Webbook
rinpol	1120.00	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1095.00	NIST Webbook
rinpol	1083.50	NIST Webbook
rinpol	1084.30	NIST Webbook
rinpol	1080.77	NIST Webbook
rinpol	1104.00	NIST Webbook
rinpol	1106.00	NIST Webbook
rinpol	1109.00	NIST Webbook
rinpol	1108.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1113.00	NIST Webbook
rinpol	1115.00	NIST Webbook
rinpol	1119.00	NIST Webbook
rinpol	1051.00	NIST Webbook
rinpol	1088.10	NIST Webbook
rinpol	1087.00	NIST Webbook
rinpol	1125.00	NIST Webbook
rinpol	1093.15	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1096.50	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1085.80	NIST Webbook
rinpol	1088.40	NIST Webbook
rinpol	1090.00	NIST Webbook
rinpol	1087.00	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1082.00	NIST Webbook
rinpol	1089.00	NIST Webbook
rinpol	1061.00	NIST Webbook
rinpol	1081.00	NIST Webbook
rinpol	1090.00	NIST Webbook
rinpol	1099.00	NIST Webbook
rinpol	1095.00	NIST Webbook
rinpol	1106.00	NIST Webbook
rinpol	1106.00	NIST Webbook
rinpol	1093.00	NIST Webbook

rinpol	1082.50		NIST Webbook
rinpol	1072.00		NIST Webbook
ripol	1368.90		NIST Webbook
ripol	1395.00		NIST Webbook
ripol	1369.00		NIST Webbook
ripol	1394.80		NIST Webbook
ripol	1390.00		NIST Webbook
ripol	1369.00		NIST Webbook
ripol	1352.00		NIST Webbook
ripol	1362.00		NIST Webbook
ripol	1364.00		NIST Webbook
ripol	1369.00		NIST Webbook
ripol	1374.00		NIST Webbook
ripol	1362.00		NIST Webbook
ripol	1430.80		NIST Webbook
ripol	1394.80		NIST Webbook
ripol	1395.00		NIST Webbook
tb	462.90	K	KDB
tc	665.10	K	KDB
tf	223.61 ± 0.20	K	NIST Webbook
vc	0.446	m3/kmol	KDB
zc	0.2364390		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.46	J/mol×K	637.55	Joback Method
cpg	310.90	J/mol×K	603.01	Joback Method
cpg	298.71	J/mol×K	568.47	Joback Method
cpg	285.86	J/mol×K	533.92	Joback Method
cpg	272.33	J/mol×K	499.38	Joback Method
cpg	258.11	J/mol×K	464.84	Joback Method
cpg	333.41	J/mol×K	672.09	Joback Method
dvisc	0.0017125	Pa×s	253.92	Joback Method
dvisc	0.0002068	Pa×s	464.84	Joback Method
dvisc	0.0002547	Pa×s	429.69	Joback Method
dvisc	0.0003255	Pa×s	394.53	Joback Method
dvisc	0.0004364	Pa×s	359.38	Joback Method
dvisc	0.0006236	Pa×s	324.23	Joback Method
dvisc	0.0009718	Pa×s	289.07	Joback Method
hvapt	49.70	kJ/mol	420.50	NIST Webbook

rhol	885.86	kg/m3	293.10	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43482e+01
Coeff. B	-3.94990e+03
Coeff. C	-6.11560e+01
Temperature range (K), min.	342.07
Temperature range (K), max.	498.25

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.31621e+01
Coeff. B	-9.06264e+03
Coeff. C	-9.75815e+00
Coeff. D	3.83702e-06
Temperature range (K), min.	223.64
Temperature range (K), max.	680.00

Sources

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/mol678.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C933982&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=678

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

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
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