Benzene, 1-ethyl-3,5-dimethyl-

Other names:	1,3-DIMETHYL-5-ETHYLBENZENE
	1-Ethyl-3,5-dimethylbenzene
	5-Ethyl-1,3-dimethylbenzene
	5-Ethyl-m-xylene
	m-Xylene, 5-ethyl-
Inchi:	InChI=1S/C10H14/c1-4-10-6-8(2)5-9(3)7-10/h5-7H,4H2,1-3H3
InchiKey:	LMAUULKNZLEMGN-UHFFFAOYSA-N
Formula:	C10H14
SMILES:	CCc1cc(C)cc(C)c1
Mol. weight [g/mol]:	134.22
CAS:	934-74-7

Physical Properties

Property code	Value	Unit	Source
chl	-5848.10 ± 1.00	kJ/mol	NIST Webbook
chl	-5848.70 ± 2.60	kJ/mol	NIST Webbook
gf	126.47	kJ/mol	Joback Method
hf	-36.14	kJ/mol	Joback Method
hfl	-87.30 ± 2.60	kJ/mol	NIST Webbook
hfl	-87.80 ± 1.20	kJ/mol	NIST Webbook
hfus	14.92	kJ/mol	Joback Method
hvap	52.40	kJ/mol	NIST Webbook
log10ws	-3.23		Crippen Method
logp	2.866		Crippen Method
mcvol	128.000	ml/mol	McGowan Method
pc	2838.39	kPa	Joback Method
rinpol	1045.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1049.75		NIST Webbook
rinpol	1050.00		NIST Webbook
rinpol	1052.20		NIST Webbook
rinpol	1048.50		NIST Webbook
rinpol	1048.20		NIST Webbook
rinpol	1049.10		NIST Webbook
rinpol	1048.00		NIST Webbook

rinpol	1053.00	NIST Webbook
rinpol	1046.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1050.00	NIST Webbook
rinpol	1050.00	NIST Webbook
rinpol	1042.60	NIST Webbook
rinpol	1042.70	NIST Webbook
rinpol	1043.50	NIST Webbook
rinpol	1046.10	NIST Webbook
rinpol	1043.46	NIST Webbook
rinpol	1069.00	NIST Webbook
rinpol	1074.00	NIST Webbook
rinpol	1079.00	NIST Webbook
rinpol	1073.00	NIST Webbook
rinpol	1080.00	NIST Webbook
rinpol	1085.00	NIST Webbook
rinpol	1089.00	NIST Webbook
rinpol	1042.70	NIST Webbook
rinpol	1048.20	NIST Webbook
rinpol	1058.20	NIST Webbook
rinpol	1043.00	NIST Webbook
rinpol	1076.00	NIST Webbook
rinpol	1049.75	NIST Webbook
rinpol	1074.00	NIST Webbook
rinpol	1043.00	NIST Webbook
rinpol	1041.30	NIST Webbook
rinpol	1041.90	NIST Webbook
rinpol	1044.03	NIST Webbook
rinpol	1044.15	NIST Webbook
rinpol	1044.00	NIST Webbook
rinpol	1040.64	NIST Webbook
rinpol	1043.33	NIST Webbook
rinpol	1045.32	NIST Webbook
rinpol	1056.96	NIST Webbook
rinpol	1060.10	NIST Webbook
rinpol	1062.45	NIST Webbook
rinpol	1043.00	NIST Webbook
rinpol	1049.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1053.00	NIST Webbook
rinpol	1051.00	NIST Webbook
rinpol	1049.00	NIST Webbook
rinpol	1048.00	NIST Webbook

rinpol	1057.00		NIST Webbook
rinpol	1061.00		NIST Webbook
rinpol	1065.90		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1044.10		NIST Webbook
rinpol	1058.00		NIST Webbook
rinpol	1058.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1049.60		NIST Webbook
rinpol	1050.00		NIST Webbook
ripol	1297.00		NIST Webbook
ripol	1319.80		NIST Webbook
ripol	1297.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1309.00		NIST Webbook
ripol	1321.00		NIST Webbook
ripol	1297.00		NIST Webbook
ripol	1347.00		NIST Webbook
ripol	1319.00		NIST Webbook
ripol	1297.00		NIST Webbook
ripol	1325.90		NIST Webbook
ripol	1320.00		NIST Webbook
tb	464.84	K	Joback Method
tc	672.09	K	Joback Method
tf	188.79 ± 0.06	K	NIST Webbook
tf	188.79 ± 0.04	K	NIST Webbook
tf	188.82 ± 0.03	K	NIST Webbook
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.46	J/mol×K	637.55	Joback Method
cpg	333.41	J/mol×K	672.09	Joback Method
cpg	258.11	J/mol×K	464.84	Joback Method
cpg	272.33	J/mol×K	499.38	Joback Method
cpg	285.86	J/mol×K	533.92	Joback Method
cpg	298.71	J/mol×K	568.47	Joback Method
cpg	310.90	J/mol×K	603.01	Joback Method
dvisc	0.0002068	Pa×s	464.84	Joback Method

dvisc	0.0002547	Pa×s	429.69	Joback Method
dvisc	0.0017125	Pa×s	253.92	Joback Method
dvisc	0.0009718	Pa×s	289.07	Joback Method
dvisc	0.0006236	Pa×s	324.23	Joback Method
dvisc	0.0004364	Pa×s	359.38	Joback Method
dvisc	0.0003255	Pa×s	394.53	Joback Method
hvapt	47.50	kJ/mol	375.50	NIST Webbook
hvapt	48.00	kJ/mol	411.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46255e+01
Coeff. B	-4.02670e+03
Coeff. C	-5.45470e+01
Temperature range (K), min.	335.39
Temperature range (K), max.	486.88

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.08217e+02
Coeff. B	-9.87144e+03
Coeff. C	-1.36532e+01
Coeff. D	7.76907e-06
Temperature range (K), min.	188.82
Temperature range (K), max.	655.00

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol682.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C934747&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=682

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

Legend

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
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