Benzene, 1-ethyl-2-methyl-

Other names:	1,2-Methylethylbenzene
	1-ETHYL-2-METHYLBENZENE
	1-METHYL-2-ETHYLBENZENE
	2-Ethylmethylbenzene
	2-Ethyltoluene
	2-Methyl-1-ethylbenzene
	2-ethyl-3-methylbenzene
	NSC 405731
	O-ETHYLMETHYLBENZENE
	Toluene, 2-ethyl-
	Toluene, o-ethyl-
	benzene, 1-methyl-2-ethyl-
	o-Ethyltoluene
	o-Methylethylbenzene
	ortho-Ethyltoluene
Inchi:	InChI=1S/C9H12/c1-3-9-7-5-4-6-8(9)2/h4-7H,3H2,1-2H3
InchiKey:	HYFLWBNQFMXCPA-UHFFFAOYSA-N
Formula:	C9H12
SMILES:	CCc1ccccc1C
Mol. weight [g/mol]:	120.19
CAS:	611-14-3

Physical Properties

Property code	Value	Unit	Source
af	0.2940		KDB
chl	-5210.17 ± 0.96	kJ/mol	NIST Webbook
gf	131.20	kJ/mol	KDB
hcg	5210.17	kJ/mol	KDB
hcn	4946.074	kJ/mol	KDB
hf	1.20 ± 1.20	kJ/mol	NIST Webbook
hf	1.21	kJ/mol	KDB
hfl	-46.50 ± 1.10	kJ/mol	NIST Webbook
hfus	12.72	kJ/mol	Joback Method
hvap	46.90	kJ/mol	NIST Webbook
hvap	47.70	kJ/mol	NIST Webbook
hvap	47.70	kJ/mol	NIST Webbook

log10ws	-3.21		Estimated Solubility Method
log10ws	-3.21		Aqueous Solubility Prediction Method
logp	2.557		Crippen Method
mcvol	113.910	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
pc	3040.00	kPa	KDB
rinpol	983.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	972.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	979.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	960.00		NIST Webbook
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rinpol	994.00		NIST Webbook
rinpol	985.50		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	971.00		NIST Webbook
rinpol	963.00		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	974.00		NIST Webbook
rinpol	963.00		NIST Webbook
rinpol	965.30		NIST Webbook
rinpol	955.00		NIST Webbook
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rinpol	150.40		NIST Webbook
rinpol	155.40		NIST Webbook

rinpol	980.00	NIST Webbook
rinpol	978.00	NIST Webbook
rinpol	151.39	NIST Webbook
rinpol	961.54	NIST Webbook
rinpol	973.50	NIST Webbook
rinpol	974.60	NIST Webbook
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rinpol	962.00	NIST Webbook
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rinpol	974.00	NIST Webbook
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rinpol	963.20	NIST Webbook
rinpol	964.70	NIST Webbook
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rinpol	969.30	NIST Webbook
rinpol	968.80	NIST Webbook
rinpol	961.20	NIST Webbook
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rinpol	969.00	NIST Webbook
rinpol	969.00	NIST Webbook
rinpol	991.00	NIST Webbook
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ripol	1258.00		NIST Webbook
ripol	1222.00		NIST Webbook
ripol	1265.00		NIST Webbook
ripol	1272.00		NIST Webbook
ripol	1300.00		NIST Webbook
ripol	1286.70		NIST Webbook
tb	438.30	K	KDB
tc	651.00	K	KDB
tf	213.55	K	Aqueous Solubility Prediction Method
tf	192.30	K	KDB
vc	0.460	m3/kmol	KDB
zc	0.2583530		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.87	J/mol×K	436.98	Joback Method
cpg	229.41	J/mol×K	471.74	Joback Method
cpg	242.24	J/mol×K	506.50	Joback Method
cpg	254.38	J/mol×K	541.26	Joback Method
cpg	265.87	J/mol×K	576.01	Joback Method
cpg	276.72	J/mol×K	610.77	Joback Method
cpg	286.96	J/mol×K	645.53	Joback Method
dvisc	0.0007303	Pa×s	299.08	Joback Method
dvisc	0.0012000	Pa×s	264.61	Joback Method
dvisc	0.0022882	Pa×s	230.13	Joback Method
dvisc	0.0004925	Pa×s	333.56	Joback Method
dvisc	0.0003576	Pa×s	368.03	Joback Method
dvisc	0.0002742	Pa×s	402.50	Joback Method
dvisc	0.0002193	Pa×s	436.98	Joback Method
hvapt	43.60	kJ/mol	398.00	NIST Webbook
rfi	1.50208		298.15	KDB

rfi	1.50450		293.15	Isobaric Vapor Liquid Equilibrium Data for the System of 1-Methyl-2-Ethylbenzene + 1,2,4-Trimethylbenzene at 10 kPa
rhol	881.00	kg/m3	293.00	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	335.50	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42140e+01
Coeff. B	-3.71914e+03
Coeff. C	-5.07440e+01
Temperature range (K), min.	317.80
Temperature range (K), max.	468.51

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.26756e+01
Coeff. B	-7.52536e+03
Coeff. C	-6.78754e+00
Coeff. D	2.05615e-06
Temperature range (K), min.	192.35
Temperature range (K), max.	651.15

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol659.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Binary Diffusion Coefficients of 2-Ethyltoluene, 3-Ethyltoluene, and 4-Ethyltoluene in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je800738n
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Isobaric Vapor Liquid Equilibrium Data for the System of 1-Methyl-2-Ethylbenzene + 1,2,4-Trimethylbenzene at 10 kPa:	https://www.doi.org/10.1021/je301122r
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=659
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C611143&Units=SI

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
hcg:	Heat of Combustion, Gross form
hcn:	Heat of Combustion, Net Form
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
nfpaf:	NFPA Fire Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility