Benzene, 1-ethyl-4-methyl-

Other names:	1,4-Methylethylbenzene
	1-ETHYL-4-METHYLBENZENE
	1-METHYL-4-ETHYLBENZENE
	4-Ethyltoluene
	4-Methylethylbenzene
	4-ethylmethylbenzene
	Benzene, 1-methyl-4-ethyl-
	NSC 74177
	P-ETHYLMETHYLBENZENE
	Toluene, p-ethyl-
	p-Ethyltoluene
	p-Methylethylbenzene
	para-Ethyltoluene
Inchi:	InChI=1S/C9H12/c1-3-9-6-4-8(2)5-7-9/h4-7H,3H2,1-2H3
InchiKey:	JRLPEMVDPFPYPJ-UHFFFAOYSA-N
Formula:	C9H12
SMILES:	CCc1ccc(C)cc1
Mol. weight [g/mol]:	120.19
CAS:	622-96-8

Physical Properties

Property code	Value	Unit	Source
af	0.3220		KDB
chl	-5206.80 ± 1.30	kJ/mol	NIST Webbook
gf	126.80	kJ/mol	KDB
hcg	5206.78	kJ/mol	KDB
hcn	4942.685	kJ/mol	KDB
hf	-3.30 ± 1.50	kJ/mol	NIST Webbook
hf	-2.05	kJ/mol	KDB
hfl	-49.90 ± 1.40	kJ/mol	NIST Webbook
hfus	12.72	kJ/mol	Joback Method
hvap	46.60	kJ/mol	NIST Webbook
hvap	46.60	kJ/mol	NIST Webbook
hvap	46.50	kJ/mol	NIST Webbook
log10ws	-3.11		Estimated Solubility Method

log10ws	-3.11		Aqueous Solubility Prediction Method
logp	2.557		Crippen Method
mcvol	113.910	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
pc	3233.00 ± 8.00	kPa	NIST Webbook
pc	3230.00 ± 100.00	kPa	NIST Webbook
pc	3230.00	kPa	KDB
pc	3173.00 ± 100.00	kPa	NIST Webbook
rinpol	147.30		NIST Webbook
rinpol	148.30		NIST Webbook
rinpol	148.90		NIST Webbook
rinpol	165.60		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	965.30		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	963.00		NIST Webbook
rinpol	962.00		NIST Webbook
rinpol	941.60		NIST Webbook
rinpol	956.80		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	951.50		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	957.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	968.50		NIST Webbook
rinpol	977.00		NIST Webbook
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ripol	1242.00		NIST Webbook
ripol	1261.00		NIST Webbook
ripol	1231.00		NIST Webbook
ripol	1201.00		NIST Webbook
ripol	1225.00		NIST Webbook
ripol	1269.00		NIST Webbook
tb	434.70 ± 2.00	K	NIST Webbook
tb	435.13 ± 0.10	K	NIST Webbook
tb	435.09 ± 0.50	K	NIST Webbook
tb	435.10 ± 0.15	K	NIST Webbook
tb	435.00 ± 1.60	K	NIST Webbook
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tc	640.20	K	KDB
tf	209.91 ± 0.50	K	NIST Webbook
tf	217.00 ± 4.00	K	NIST Webbook
tf	208.99 ± 0.20	K	NIST Webbook
tf	210.80	K	KDB
tf	211.05	K	Aqueous Solubility Prediction Method
tf	210.79 ± 0.10	K	NIST Webbook
tf	209.08 ± 0.20	K	NIST Webbook
tf	209.91 ± 0.60	K	NIST Webbook
tf	208.99 ± 1.00	K	NIST Webbook
tf	209.14 ± 0.20	K	NIST Webbook
tf	210.55 ± 0.40	K	NIST Webbook
tf	210.78 ± 0.20	K	NIST Webbook
tf	210.75 ± 0.03	K	NIST Webbook
tf	210.78 ± 0.02	K	NIST Webbook
tf	210.80 ± 0.01	K	NIST Webbook
vc	0.470	m3/kmol	KDB
zc	0.2851990		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.38	J/mol×K	541.26	Joback Method
cpg	286.96	J/mol×K	645.53	Joback Method
cpg	276.72	J/mol×K	610.77	Joback Method
cpg	265.87	J/mol×K	576.01	Joback Method
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

dvisc	0.0002193	Pa×s	436.98	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	0.0022882	Pa×s	230.13	Joback Method
dvisc	0.0012000	Pa×s	264.61	Joback Method
dvisc	0.0007303	Pa×s	299.08	Joback Method
hvapt	43.20	kJ/mol	395.50	NIST Webbook
rfi	1.49244		298.15	KDB
rhol	861.07	kg/m3	293.15	Isobaric VLE data for 1-methyl-3-ethylbenzene or 1-methyl-4-ethylbenzene + 1,2,4-trimethylbenzene at 20 kPa
rhol	861.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42141e+01
Coeff. B	-3.63868e+03
Coeff. C	-5.59640e+01
Temperature range (K), min.	317.24
Temperature range (K), max.	464.68

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.21809e+01
Coeff. B	-8.31456e+03
Coeff. C	-9.76149e+00
Coeff. D	4.68582e-06
Temperature range (K), min.	210.83
Temperature range (K), max.	640.15

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=661
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Binary Diffusion Coefficients of 2-Ethyltoluene, 3-Ethyltoluene, and 4-Ethyltoluene in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je800738n
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C622968&Units=SI
Isobaric VLE data for 1-methyl-3-ethylbenzene or 1-methyl-4-ethylbenzene + 1,2,4-trimethylbenzene at 20 kPa:	https://www.doi.org/10.1016/j.jct.2013.01.016
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://www.cheric.org/files/research/kdb/mol/mol661.mol
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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https://www.chemeo.com/cid/32-701-7/Benzene-1-ethyl-4-methyl.pdf
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