

Benzene, 1-ethyl-3-methyl-

Other names:	1,3-Methylethylbenzene
	1,3-ethylmethylbenzene
	1-ETHYL-3-METHYLBENZENE
	1-METHYL-3-ETHYLBENZENE
	3-Ethyl-1-methylbenzene
	3-Ethylmethylbenzene
	3-Ethyltoluene
	3-Methylethylbenzene
	Benzene, 3-ethyl-1-methyl-
	M-ETHYLMETHYLBENZENE
	NSC 74176
	Toluene, m-ethyl-
	benzene, 1-methyl-3-ethyl-
	m-Ethyltoluene
	m-Methylethylbenzene

Inchi:	InChI=1S/C9H12/c1-3-9-6-4-5-8(2)7-9/h4-7H,3H2,1-2H3
InchiKey:	ZLCSFXXPPANWQY-UHFFFAOYSA-N
Formula:	C9H12
SMILES:	CCc1cccc(C)c1
Mol. weight [g/mol]:	120.19
CAS:	620-14-4

Physical Properties

Property code	Value	Unit	Source
af	0.3600		KDB
chl	-5207.90 ± 1.10	kJ/mol	NIST Webbook
gf	126.50	kJ/mol	KDB
hcg	5207.87	kJ/mol	KDB
hcn	4943.773	kJ/mol	KDB
hf	-1.90 ± 1.20	kJ/mol	NIST Webbook
hf	-1.93	kJ/mol	KDB
hfl	-48.80 ± 1.20	kJ/mol	NIST Webbook
hfus	12.72	kJ/mol	Joback Method
hvap	46.60	kJ/mol	NIST Webbook
hvap	46.90	kJ/mol	NIST Webbook
hvap	46.90	kJ/mol	NIST Webbook

log10ws	-2.75		Crippen Method
logp	2.557		Crippen Method
mcvol	113.910	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
pc	2840.00	kPa	KDB
rinpol	147.30		NIST Webbook
rinpol	958.60		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	145.20		NIST Webbook
rinpol	958.00		NIST Webbook
rinpol	946.70		NIST Webbook
rinpol	145.20		NIST Webbook
rinpol	946.00		NIST Webbook
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rinpol	948.70		NIST Webbook
rinpol	950.00		NIST Webbook
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rinpol	970.00		NIST Webbook
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ripol	1248.10		NIST Webbook
ripol	1235.00		NIST Webbook
ripol	1218.00		NIST Webbook
ripol	1216.00		NIST Webbook
ripol	1203.30		NIST Webbook
ripol	1219.10		NIST Webbook
ripol	1224.90		NIST Webbook
ripol	1202.00		NIST Webbook
tb	435.20 ± 2.00	K	NIST Webbook
tb	431.70	K	NIST Webbook
tb	432.70 ± 2.00	K	NIST Webbook

tb	431.00 ± 4.00	K	NIST Webbook
tb	434.70 ± 0.20	K	NIST Webbook
tb	434.60 ± 0.20	K	NIST Webbook
tb	434.60 ± 0.20	K	NIST Webbook
tb	434.60 ± 0.20	K	NIST Webbook
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tb	434.60 ± 1.00	K	NIST Webbook
tb	434.44 ± 0.20	K	NIST Webbook
tb	434.00 ± 3.00	K	NIST Webbook
tb	432.00 ± 4.00	K	NIST Webbook
tb	435.85 ± 1.50	K	NIST Webbook
tb	434.50	K	NIST Webbook
tb	434.44 ± 0.20	K	NIST Webbook
tc	637.00	K	KDB
tf	177.60	K	KDB
vc	0.490	m3/kmol	KDB
zc	0.2627470		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	43.40	kJ/mol	393.00	NIST Webbook
rfi	1.49406		298.15	KDB
rhoI	865.00	kg/m3	293.00	KDB
rhoI	864.44	kg/m3	293.15	Isobaric VLE data for 1-methyl-3-ethylbenzene or 1-methyl-4-ethylbenzene + 1,2,4-trimethylbenzene at 20 kPa

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42689e+01
Coeff. B	-3.70876e+03
Coeff. C	-5.01780e+01
Temperature range (K), min.	315.44
Temperature range (K), max.	464.22

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	7.56008e+01
Coeff. B	-8.01685e+03
Coeff. C	-8.76798e+00
Coeff. D	3.83709e-06
Temperature range (K), min.	177.61
Temperature range (K), max.	637.15

Sources

Binary Diffusion Coefficients of
2-Ethyltoluene, 3-Ethyltoluene, and
4-Ethyltoluene in Supercritical Carbon
Dioxide:
The Yaws Handbook of Vapor
Pressure:
Isobaric VLE data for
1-methyl-3-ethylbenzene or
McGowan Method
1-methyl-4-ethylbenzene +
1,2,4-trimethylbenzene at 20 kPa:
Crippen Method:

NIST Webbook:

Crippen Method:

Joback Method:

KDB:

<https://www.doi.org/10.1021/je800738n>

<https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=660>

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<https://www.doi.org/10.1016/j.jct.2013.01.016>

<http://link.springer.com/article/10.1007/BF02311772>

https://www.chemeo.com/doc/models/crippen_log10ws

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C620144&Units=SI>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

https://en.wikipedia.org/wiki/Joback_method

<https://www.cheric.org/files/research/kdb/mol/mol660.mol>

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
rhof:	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

Latest version available from:

<https://www.chemeo.com/cid/28-057-8/Benzene-1-ethyl-3-methyl.pdf>

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