Benzene, 1-ethyl-2,4-dimethyl-

Other names:	1,3-DIMETHYL-4-ETHYLBENZENE
	1-Ethyl-2,4-dimethylbenzene
	2,4-Dimethyl-1-ethylbenzene
	4-ETHYL-M-XYLENE
	4-Ethyl-1,3-dimethylbenzene
	m-Xylene, 4-ethyl-
Inchi:	InChI=1S/C10H14/c1-4-10-6-5-8(2)7-9(10)3/h5-7H,4H2,1-3H3
InchiKey:	MEMBJMDZWKVOTB-UHFFFAOYSA-N
Formula:	C10H14
SMILES:	CCc1ccc(C)cc1C
Mol. weight [g/mol]:	134.22
CAS:	874-41-9

Physical Properties

Property code	Value	Unit	Source
chl	-5851.80 ± 1.10	kJ/mol	NIST Webbook
gf	126.47	kJ/mol	Joback Method
hf	-36.14	kJ/mol	Joback Method
hfl	-84.10 ± 1.30	kJ/mol	NIST Webbook
hfus	14.92	kJ/mol	Joback Method
hvap	53.30	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	1034.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1061.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1083.50		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1067.00		NIST Webbook
rinpol	1069.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1064.00		NIST Webbook

rinpol	1071.00	NIST Webbook
rinpol	1075.00	NIST Webbook
rinpol	1064.00	NIST Webbook
rinpol	1070.80	NIST Webbook
rinpol	1074.20	NIST Webbook
rinpol	1068.00	NIST Webbook
rinpol	1069.00	NIST Webbook
rinpol	1069.00	NIST Webbook
rinpol	1068.70	NIST Webbook
rinpol	1069.60	NIST Webbook
rinpol	1069.00	NIST Webbook
rinpol	1075.00	NIST Webbook
rinpol	1096.00	NIST Webbook
rinpol	1069.00	NIST Webbook
rinpol	1069.00	NIST Webbook
rinpol	1070.00	NIST Webbook
rinpol	1071.00	NIST Webbook
rinpol	1061.70	NIST Webbook
rinpol	1061.80	NIST Webbook
rinpol	1066.00	NIST Webbook
rinpol	1060.40	NIST Webbook
rinpol	1085.00	NIST Webbook
rinpol	1089.00	NIST Webbook
rinpol	1093.00	NIST Webbook
rinpol	1065.00	NIST Webbook
rinpol	1080.00	NIST Webbook
rinpol	1078.00	NIST Webbook
rinpol	1066.60	NIST Webbook
rinpol	1070.80	NIST Webbook
rinpol	1077.80	NIST Webbook
rinpol	1062.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1069.60	NIST Webbook
rinpol	1069.00	NIST Webbook
rinpol	1070.00	NIST Webbook
rinpol	1073.00	NIST Webbook
rinpol	1070.80	NIST Webbook
rinpol	1086.60	NIST Webbook
rinpol	1075.00	NIST Webbook
rinpol	1063.00	NIST Webbook
rinpol	1063.94	NIST Webbook
rinpol	1064.79	NIST Webbook
rinpol	1065.00	NIST Webbook
rinpol	1062.00	NIST Webbook

rinpol	1076.67		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1075.00		NIST Webbook
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rinpol	1075.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1060.50		NIST Webbook
rinpol	1075.00		NIST Webbook
ripol	1342.80		NIST Webbook
ripol	1316.00		NIST Webbook
ripol	1350.00		NIST Webbook
ripol	1316.00		NIST Webbook
ripol	1346.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1350.00		NIST Webbook
ripol	1348.00		NIST Webbook
ripol	1348.00		NIST Webbook
ripol	1326.00		NIST Webbook
ripol	1373.00		NIST Webbook
ripol	1347.00		NIST Webbook
ripol	1348.00		NIST Webbook
tb	464.84	K	Joback Method
tc	672.09	K	Joback Method
tf	210.27 ± 0.02	K	NIST Webbook
tf	210.14 ± 0.20	K	NIST Webbook
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	322.46	J/mol×K	637.55	Joback Method

cpg	333.41	J/mol×K	672.09	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
dvisc	0.0002547	Pa×s	429.69	Joback Method
dvisc	0.0002068	Pa×s	464.84	Joback Method
hvapt	48.50	kJ/mol	415.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48165e+01
Coeff. B	-4.24584e+03
Coeff. C	-4.52570e+01
Temperature range (K), min.	337.49
Temperature range (K), max.	491.95

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.98927e+01
Coeff. B	-7.79291e+03
Coeff. C	-6.32939e+00
Coeff. D	2.04034e-06
Temperature range (K), min.	210.27
Temperature range (K), max.	665.00

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/research/kdb/hcprop/showprop.php?cmpid=681

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C874419&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=681
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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