Benzene, 2-ethyl-1,3-dimethyl-

Other names:	1,3-DIMETHYL-2-ETHYLBENZENE
	2-Ethyl-1,3-dimethylbenzene
	2-ethyl-m-xylene
	m-Xylene, 2-ethyl-
Inchi:	InChI=1S/C10H14/c1-4-10-8(2)6-5-7-9(10)3/h5-7H,4H2,1-3H3
InchiKey:	CHIKRULMSSADAF-UHFFFAOYSA-N
Formula:	C10H14
SMILES:	CCc1c(C)cccc1C
Mol. weight [g/mol]:	134.22
CAS:	2870-04-4

Physical Properties

Property code	Value	Unit	Source
af	0.4050		KDB
chl	-5855.80 ± 1.10	kJ/mol	NIST Webbook
chl	-5853.00 ± 2.60	kJ/mol	NIST Webbook
gf	126.47	kJ/mol	Joback Method
hf	-36.14	kJ/mol	Joback Method
hfl	-80.10 ± 1.30	kJ/mol	NIST Webbook
hfl	-83.00 ± 2.60	kJ/mol	NIST Webbook
hfus	14.92	kJ/mol	Joback Method
hvap	53.90	kJ/mol	NIST Webbook
log10ws	-3.23		Crippen Method
logp	2.866		Crippen Method
mcvol	128.000	ml/mol	McGowan Method
pc	2929.00	kPa	KDB
rinpol	1082.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1081.60		NIST Webbook
rinpol	1084.70		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1069.60		NIST Webbook
rinpol	1064.97		NIST Webbook
rinpol	1070.40		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1099.20		NIST Webbook

rinpol	1073.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1080.75		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1081.80		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1072.10		NIST Webbook
rinpol	1075.70		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1097.10		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1061.00		NIST Webbook
ripol	1372.00		NIST Webbook
ripol	1372.10		NIST Webbook
ripol	1348.00		NIST Webbook
ripol	1363.00		NIST Webbook
ripol	1372.10		NIST Webbook
ripol	1347.50		NIST Webbook
ripol	1363.00		NIST Webbook
ripol	1348.00		NIST Webbook
ripol	1348.00		NIST Webbook
ripol	1372.00		NIST Webbook
ripol	1355.00		NIST Webbook
tb	463.10 ± 0.30	K	NIST Webbook
tb	463.16 ± 0.20	K	NIST Webbook

tb	463.10 ± 0.15	K	NIST Webbook
tb	463.10 ± 0.30	K	NIST Webbook
tb	463.10 ± 0.20	K	NIST Webbook
tb	463.20 ± 1.00	K	NIST Webbook
tb	463.16 ± 0.20	K	NIST Webbook
tb	463.20	K	NIST Webbook
tb	456.90	K	KDB
tc	665.10	K	KDB
tf	256.81 ± 0.20	K	NIST Webbook
vc	0.446	m3/kmol	KDB
zc	0.2363340		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.46	J/mol×K	637.55	Joback Method
cpg	298.71	J/mol×K	568.47	Joback Method
cpg	285.86	J/mol×K	533.92	Joback Method
cpg	272.33	J/mol×K	499.38	Joback Method
cpg	258.11	J/mol×K	464.84	Joback Method
cpg	310.90	J/mol×K	603.01	Joback Method
cpg	333.41	J/mol×K	672.09	Joback Method
dvisc	0.0017125	Pa×s	253.92	Joback Method
dvisc	0.0002068	Pa×s	464.84	Joback Method
dvisc	0.0002547	Pa×s	429.69	Joback Method
dvisc	0.0003255	Pa×s	394.53	Joback Method
dvisc	0.0004364	Pa×s	359.38	Joback Method
dvisc	0.0006236	Pa×s	324.23	Joback Method
dvisc	0.0009718	Pa×s	289.07	Joback Method
hvapt	48.80	kJ/mol	417.00	NIST Webbook
hvapt	48.60	kJ/mol	380.00	NIST Webbook
rhol	885.86	kg/m3	293.10	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.45844e+01
Coeff. B	-4.00908e+03
Coeff. C	-6.09150e+01
Temperature range (K), min.	341.33
Temperature range (K), max.	493.26

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.01218e+02
Coeff. B	-9.75905e+03
Coeff. C	-1.25287e+01
Coeff. D	6.40530e-06
Temperature range (K), min.	256.89
Temperature range (K), max.	671.00

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol680.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2870044&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=680
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

af:	Acentric Factor
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
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