Benzene, 1,3-diethyl-

Other names:	1,3-DIETHYLBENZENE
	Benzene, m-diethyl-
	m-Diethylbenzene
	meta-Diethylbenzene
Inchi:	InChI=1S/C10H14/c1-3-9-6-5-7-10(4-2)8-9/h5-8H,3-4H2,1-2H3
InchiKey:	AFZZYIJIWUTJFO-UHFFFAOYSA-N
Formula:	C10H14
SMILES:	CCc1cccc(CC)c1
Mol. weight [g/mol]:	134.22
CAS:	141-93-5

Physical Properties

Property code	Value	Unit	Source
af	0.3590		KDB
chl	-5863.00 ± 1.80	kJ/mol	NIST Webbook
chl	-5862.41 ± 0.92	kJ/mol	NIST Webbook
gf	136.10	kJ/mol	Joback Method
hf	-24.67	kJ/mol	Joback Method
hfl	-73.00 ± 1.80	kJ/mol	NIST Webbook
hfl	-73.50 ± 1.10	kJ/mol	NIST Webbook
hfus	15.31	kJ/mol	Joback Method
hvap	52.50	kJ/mol	NIST Webbook
ie	8.49 ± 0.01	eV	NIST Webbook
ie	8.49	eV	NIST Webbook
log10ws	-3.08		Crippen Method
logp	2.811		Crippen Method
mcvol	128.000	ml/mol	McGowan Method
pc	2930.00	kPa	KDB
rinpol	1034.64		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1025.70		NIST Webbook
rinpol	1028.10		NIST Webbook
rinpol	1040.40		NIST Webbook
rinpol	1045.30		NIST Webbook
rinpol	1050.70		NIST Webbook
rinpol	1031.50		NIST Webbook
rinpol	1023.20		NIST Webbook

rinpol	1025.70	NIST Webbook
rinpol	1028.10	NIST Webbook
rinpol	1027.00	NIST Webbook
rinpol	1023.18	NIST Webbook
rinpol	1032.95	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	1053.00	NIST Webbook
rinpol	1055.00	NIST Webbook
rinpol	1056.00	NIST Webbook
rinpol	1032.00	NIST Webbook
rinpol	1032.30	NIST Webbook
rinpol	1031.50	NIST Webbook
rinpol	1028.90	NIST Webbook
rinpol	1025.00	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	1033.00	NIST Webbook
rinpol	1055.00	NIST Webbook
rinpol	1039.90	NIST Webbook
rinpol	1039.00	NIST Webbook
rinpol	1032.00	NIST Webbook
rinpol	1037.00	NIST Webbook
rinpol	1056.00	NIST Webbook
rinpol	1040.00	NIST Webbook
rinpol	1055.20	NIST Webbook
rinpol	1045.00	NIST Webbook
rinpol	1034.10	NIST Webbook
rinpol	1034.43	NIST Webbook
rinpol	1045.00	NIST Webbook
rinpol	1035.00	NIST Webbook
rinpol	1033.00	NIST Webbook
rinpol	1049.74	NIST Webbook
rinpol	1040.00	NIST Webbook
rinpol	1051.00	NIST Webbook
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rinpol	1035.00	NIST Webbook
rinpol	1040.00	NIST Webbook
rinpol	1038.50	NIST Webbook
rinpol	1039.00	NIST Webbook
rinpol	1028.80	NIST Webbook
rinpol	1033.00	NIST Webbook
rinpol	1034.00	NIST Webbook
rinpol	186.60	NIST Webbook
rinpol	1036.00	NIST Webbook
rinpol	1034.80	NIST Webbook
rinpol	1036.00	NIST Webbook
rinpol	1041.00	NIST Webbook
rinpol	1038.00	NIST Webbook
rinpol	1040.00	NIST Webbook
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rinpol	1040.00	NIST Webbook
rinpol	1040.00	NIST Webbook
rinpol	1040.00	NIST Webbook
rinpol	1038.50	NIST Webbook
rinpol	1030.00	NIST Webbook
rinpol	1050.00	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	1030.00	NIST Webbook
ripol	1289.40	NIST Webbook
ripol	1309.00	NIST Webbook
ripol	1320.00	NIST Webbook
ripol	1332.00	NIST Webbook
ripol	1348.00	NIST Webbook
ripol	1298.00	NIST Webbook
ripol	1276.00	NIST Webbook

ripol	1339.00		NIST Webbook
ripol	1297.00		NIST Webbook
ripol	1276.00		NIST Webbook
ripol	1297.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1296.00		NIST Webbook
ripol	1314.00		NIST Webbook
ripol	1296.00		NIST Webbook
ripol	1310.00		NIST Webbook
ripol	1301.00		NIST Webbook
ripol	1275.80		NIST Webbook
ripol	1297.30		NIST Webbook
ripol	1275.80		NIST Webbook
ripol	1308.00		NIST Webbook
ripol	1302.00		NIST Webbook
tb	454.30	K	KDB
tc	663.60	K	KDB
tf	189.06 ± 0.15	K	NIST Webbook
tf	189.00	K	KDB
tf	189.33 ± 0.20	K	NIST Webbook
tf	189.16 ± 0.20	K	NIST Webbook
vc	0.487	m3/kmol	KDB
zc	0.2588800		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.39	J/mol×K	665.78	Joback Method
cpg	257.29	J/mol×K	459.86	Joback Method
cpg	271.96	J/mol×K	494.18	Joback Method
cpg	285.87	J/mol×K	528.50	Joback Method
cpg	299.03	J/mol×K	562.82	Joback Method
cpg	311.49	J/mol×K	597.14	Joback Method
cpg	323.27	J/mol×K	631.46	Joback Method
dvisc	0.0002163	Pa×s	459.86	Joback Method
dvisc	0.0024545	Pa×s	241.40	Joback Method
dvisc	0.0012559	Pa×s	277.81	Joback Method
dvisc	0.0007506	Pa×s	314.22	Joback Method
dvisc	0.0004992	Pa×s	350.63	Joback Method
dvisc	0.0003585	Pa×s	387.04	Joback Method
dvisc	0.0002725	Pa×s	423.45	Joback Method

hvapt	45.80	kJ/mol	412.50	NIST Webbook
hvapt	39.37	kJ/mol	454.30	KDB
rfi	1.49310		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43625e+01
Coeff. B	-3.88665e+03
Coeff. C	-5.54190e+01
Temperature range (K), min.	331.56
Temperature range (K), max.	484.84

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.37996e+01
Coeff. B	-8.84380e+03
Coeff. C	-9.89795e+00
Coeff. D	4.12081e-06
Temperature range (K), min.	189.26
Temperature range (K), max.	663.00

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol676.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C141935&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=676

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
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