Benzene, 1,2-diethyl-

Other names:	1,2-DIETHYLBENZENE
	1,2-Diethylbenzene
	Benzene, o-diethyl-
	o-Diethylbenzene
	ortho-Diethylbenzene
Inchi:	InChI=1S/C10H14/c1-3-9-7-5-6-8-10(9)4-2/h5-8H,3-4H2,1-2H3
InchiKey:	KVNYFPKFSJIPBJ-UHFFFAOYSA-N
Formula:	C10H14
SMILES:	CCc1ccccc1CC
Mol. weight [g/mol]:	134.22
CAS:	135-01-3

Physical Properties

Property code	Value	Unit	Source
af	0.3540		KDB
chl	-5867.43 ± 0.88	kJ/mol	NIST Webbook
chl	-5865.10 ± 1.80	kJ/mol	NIST Webbook
gf	136.10	kJ/mol	Joback Method
hf	-24.67	kJ/mol	Joback Method
hfl	-70.90 ± 1.80	kJ/mol	NIST Webbook
hfl	-68.50 ± 1.00	kJ/mol	NIST Webbook
hfus	15.31	kJ/mol	Joback Method
hvap	52.80	kJ/mol	NIST Webbook
ie	8.51	eV	NIST Webbook
ie	8.51	eV	NIST Webbook
log10ws	-3.28		Aqueous Solubility Prediction Method
log10ws	-3.28		Estimated Solubility Method
logp	2.811		Crippen Method
mcvol	128.000	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=2)		KDB
pc	2990.00	kPa	KDB
rinpol	1051.00		NIST Webbook
rinpol	1034.80		NIST Webbook
rinpol	1038.10		NIST Webbook

rinpol	1052.70	NIST Webbook
rinpol	1058.90	NIST Webbook
rinpol	1065.90	NIST Webbook
rinpol	1042.70	NIST Webbook
rinpol	1033.00	NIST Webbook
rinpol	1034.80	NIST Webbook
rinpol	1038.10	NIST Webbook
rinpol	1046.00	NIST Webbook
rinpol	1042.70	NIST Webbook
rinpol	1039.10	NIST Webbook
rinpol	1043.60	NIST Webbook
rinpol	1036.00	NIST Webbook
rinpol	1067.00	NIST Webbook
rinpol	1051.70	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1049.00	NIST Webbook
rinpol	1056.00	NIST Webbook
rinpol	1056.70	NIST Webbook
rinpol	1055.00	NIST Webbook
rinpol	1043.30	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	1044.00	NIST Webbook
rinpol	1044.00	NIST Webbook
rinpol	1059.00	NIST Webbook
rinpol	1050.00	NIST Webbook
rinpol	1053.00	NIST Webbook
rinpol	1053.00	NIST Webbook
rinpol	1059.00	NIST Webbook
rinpol	1059.00	NIST Webbook
rinpol	1029.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1057.00	NIST Webbook
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rinpol	1052.00	NIST Webbook
rinpol	1052.00	NIST Webbook
rinpol	1068.80	NIST Webbook
rinpol	1042.00	NIST Webbook
rinpol	1042.00	NIST Webbook
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rinpol	1088.00	NIST Webbook
rinpol	1044.00	NIST Webbook
rinpol	1066.00	NIST Webbook

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rinpol	1052.00		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1051.50		NIST Webbook
rinpol	1058.70		NIST Webbook
rinpol	1055.80		NIST Webbook
rinpol	1057.20		NIST Webbook
rinpol	1039.30		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1053.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1043.50		NIST Webbook
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rinpol	1051.00		NIST Webbook
rinpol	1057.90		NIST Webbook
rinpol	1051.80		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1053.00		NIST Webbook
ripol	1324.00		NIST Webbook
ripol	1372.00		NIST Webbook
ripol	1324.00		NIST Webbook
ripol	1299.00		NIST Webbook
ripol	1324.00		NIST Webbook
ripol	1308.50		NIST Webbook
ripol	1285.00		NIST Webbook
ripol	1299.00		NIST Webbook
ripol	1379.00		NIST Webbook
ripol	1363.00		NIST Webbook
ripol	1350.00		NIST Webbook
ripol	1337.00		NIST Webbook
ripol	1324.00		NIST Webbook
ripol	1335.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1298.80		NIST Webbook
ripol	1298.80		NIST Webbook
ripol	1289.00		NIST Webbook
tb	457.00 ± 2.00	K	NIST Webbook
tb	457.00	K	KDB

tb	456.45 ± 0.20	K	NIST Webbook
tb	456.45 ± 0.20	K	NIST Webbook
tb	456.57 ± 0.03	K	NIST Webbook
tb	456.45 ± 0.30	K	NIST Webbook
tb	456.90 ± 2.00	K	NIST Webbook
tb	449.70 ± 1.00	K	NIST Webbook
tb	454.35 ± 0.30	K	NIST Webbook
tb	456.70 ± 0.50	K	NIST Webbook
tb	456.45 ± 0.30	K	NIST Webbook
tb	457.40 ± 1.00	K	NIST Webbook
tb	456.00 ± 2.00	K	NIST Webbook
tb	450.00 ± 7.00	K	NIST Webbook
tb	456.70	K	NIST Webbook
tb	456.00 ± 2.00	K	NIST Webbook
tc	669.60	K	KDB
tf	242.00	K	KDB
tf	242.08	K	Aqueous Solubility Prediction Method
tf	241.71 ± 0.20	K	NIST Webbook
vc	0.487	m3/kmol	KDB
zc	0.2618150		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.49	J/mol×K	597.14	Joback Method
cpg	334.39	J/mol×K	665.78	Joback Method
cpg	323.27	J/mol×K	631.46	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
dvisc	0.0002163	Pa×s	459.86	Joback Method
dvisc	0.0003585	Pa×s	387.04	Joback Method
dvisc	0.0002725	Pa×s	423.45	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
hvapt	46.00	kJ/mol	416.50	NIST Webbook
hvapt	39.41	kJ/mol	457.00	KDB

rfi	1.50106	298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42021e+01
Coeff. B	-3.77470e+03
Coeff. C	-6.27460e+01
Temperature range (K), min.	334.02
Temperature range (K), max.	487.32

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.81349e+01
Coeff. B	-8.61176e+03
Coeff. C	-9.03986e+00
Coeff. D	3.36428e-06
Temperature range (K), min.	241.93
Temperature range (K), max.	668.00

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

KDB: https://www.cheric.org/files/research/kdb/mol/mol675.mol

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

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=675

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C135013&Units=SI

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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
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