

Benzene, 1,4-diethyl-

Other names:	1,4-DIETHYLBENZENE Benzene, p-diethyl- p-Diethylbenzene p-Ethylethylbenzene para-Diethylbenzene
Inchi:	InChI=1S/C10H14/c1-3-9-5-7-10(4-2)8-6-9/h5-8H,3-4H2,1-2H3
InchiKey:	DSNHSQKRULAAEI-UHFFFAOYSA-N
Formula:	C10H14
SMILES:	CCc1ccc(CC)cc1
Mol. weight [g/mol]:	134.22
CAS:	105-05-5

Physical Properties

Property code	Value	Unit	Source
af	0.4040		KDB
chl	-5863.08 ± 0.79	kJ/mol	NIST Webbook
chl	-5862.90 ± 1.80	kJ/mol	NIST Webbook
gf	136.10	kJ/mol	Joback Method
hf	-24.67	kJ/mol	Joback Method
hfl	-73.10 ± 1.80	kJ/mol	NIST Webbook
hfl	-72.84 ± 0.96	kJ/mol	NIST Webbook
hfus	15.31	kJ/mol	Joback Method
hvap	52.50	kJ/mol	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.43	eV	NIST Webbook
log10ws	-3.75		Estimated Solubility Method
log10ws	-3.75		Aqueous Solubility Prediction Method
logp	2.811		Crippen Method
mcvol	128.000	ml/mol	McGowan Method
pc	2803.00 ± 7.00	kPa	NIST Webbook
pc	2800.00 ± 40.00	kPa	NIST Webbook
pc	2803.00	kPa	KDB
rinpol	1037.00		NIST Webbook
rinpol	1055.00		NIST Webbook

rinpol	1066.00	NIST Webbook
rinpol	1029.00	NIST Webbook
rinpol	1080.00	NIST Webbook
rinpol	1036.33	NIST Webbook
rinpol	1040.00	NIST Webbook
rinpol	1040.00	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	1040.70	NIST Webbook
rinpol	1039.00	NIST Webbook
rinpol	1038.00	NIST Webbook
rinpol	1041.00	NIST Webbook
rinpol	1043.00	NIST Webbook
rinpol	1051.00	NIST Webbook
rinpol	1069.00	NIST Webbook
rinpol	1045.00	NIST Webbook
rinpol	1045.00	NIST Webbook
rinpol	1053.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1042.00	NIST Webbook
rinpol	1053.00	NIST Webbook
rinpol	1053.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1046.00	NIST Webbook
rinpol	1044.00	NIST Webbook
rinpol	1039.00	NIST Webbook
rinpol	1060.01	NIST Webbook
rinpol	1057.31	NIST Webbook
rinpol	1053.74	NIST Webbook
rinpol	1042.04	NIST Webbook
rinpol	1042.00	NIST Webbook
rinpol	1043.00	NIST Webbook
rinpol	1039.17	NIST Webbook
rinpol	1084.00	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	1046.00	NIST Webbook
rinpol	1046.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1040.00	NIST Webbook
rinpol	1040.00	NIST Webbook
rinpol	1058.00	NIST Webbook
rinpol	1042.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1053.00	NIST Webbook

rinpol	1059.00	NIST Webbook
rinpol	1036.80	NIST Webbook
rinpol	1039.30	NIST Webbook
rinpol	1047.90	NIST Webbook
rinpol	1053.40	NIST Webbook
rinpol	1059.30	NIST Webbook
rinpol	1037.10	NIST Webbook
rinpol	1033.80	NIST Webbook
rinpol	1036.80	NIST Webbook
rinpol	1039.30	NIST Webbook
rinpol	1040.00	NIST Webbook
rinpol	1033.82	NIST Webbook
rinpol	1032.00	NIST Webbook
rinpol	1036.70	NIST Webbook
rinpol	1036.70	NIST Webbook
rinpol	1037.10	NIST Webbook
rinpol	1039.10	NIST Webbook
rinpol	1055.00	NIST Webbook
rinpol	1039.00	NIST Webbook
rinpol	1068.00	NIST Webbook
rinpol	1045.25	NIST Webbook
rinpol	1042.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1046.80	NIST Webbook
rinpol	1070.10	NIST Webbook
rinpol	1056.00	NIST Webbook
rinpol	1040.50	NIST Webbook
rinpol	1040.66	NIST Webbook
rinpol	1040.69	NIST Webbook
rinpol	1041.00	NIST Webbook
rinpol	1036.00	NIST Webbook
rinpol	1036.00	NIST Webbook
rinpol	1030.00	NIST Webbook
ripol	1283.60	NIST Webbook
ripol	1291.50	NIST Webbook
ripol	1305.00	NIST Webbook
ripol	1284.00	NIST Webbook
ripol	1305.00	NIST Webbook
ripol	1353.00	NIST Webbook
ripol	1284.00	NIST Webbook
ripol	1307.00	NIST Webbook
ripol	1306.00	NIST Webbook
ripol	1305.00	NIST Webbook
ripol	1300.00	NIST Webbook

ripol	1283.60		NIST Webbook
ripol	1315.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1312.00		NIST Webbook
ripol	1293.00		NIST Webbook
ripol	1305.20		NIST Webbook
ripol	1289.40		NIST Webbook
tb	456.90 ± 0.30	K	NIST Webbook
tb	456.75 ± 0.20	K	NIST Webbook
tb	457.00	K	NIST Webbook
tb	456.15 ± 2.00	K	NIST Webbook
tb	456.89 ± 0.30	K	NIST Webbook
tb	456.80 ± 0.50	K	NIST Webbook
tb	456.94	K	KDB
tb	456.91 ± 0.30	K	NIST Webbook
tb	457.00 ± 0.60	K	NIST Webbook
tb	456.90 ± 0.20	K	NIST Webbook
tb	456.90 ± 0.15	K	NIST Webbook
tb	456.00 ± 2.00	K	NIST Webbook
tb	456.90 ± 0.03	K	NIST Webbook
tb	456.75 ± 0.20	K	NIST Webbook
tb	457.00 ± 2.00	K	NIST Webbook
tb	456.90 ± 1.00	K	NIST Webbook
tb	456.75 ± 0.30	K	NIST Webbook
tb	456.00 ± 2.00	K	NIST Webbook
tb	456.80 ± 0.20	K	NIST Webbook
tb	457.00 ± 2.00	K	NIST Webbook
tc	657.90	K	KDB
tc	657.90 ± 0.50	K	NIST Webbook
tc	657.89 ± 0.15	K	NIST Webbook
tc	657.87 ± 0.03	K	NIST Webbook
tf	230.32	K	KDB
tf	230.21	K	Aqueous Solubility Prediction Method
tf	229.90 ± 0.20	K	NIST Webbook
tf	229.60 ± 0.60	K	NIST Webbook
vc	0.480	m3/kmol	KDB
zc	0.2462180		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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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	45.80	kJ/mol	416.50	NIST Webbook
hvapt	39.37	kJ/mol	456.90	KDB
rfi	1.49245		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.45880e+01
Coeff. B	-4.01384e+03
Coeff. C	-5.43350e+01
Temperature range (K), min.	335.02
Temperature range (K), max.	487.02

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	8.43431e+01
Coeff. B	-8.82443e+03
Coeff. C	-1.00236e+01
Coeff. D	4.67268e-06
Temperature range (K), min.	230.32
Temperature range (K), max.	657.96

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=677
Liquid Liquid Equilibria of the Ternary Systems Undecane + 1,4-Dichlorobenzene + 1,4-Dibromobenzene + Tetrahydrothiophene 1,1-Dioxide and The Yaws Handbook of Vapor Pressure	https://www.doi.org/10.1021/je200465z
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Undecane + 1,4-Dichlorobenzene + Tetrahydrothiophene 1,1-Dioxide at T= (323.15, 348.15, and 373.15) K:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
Aqueous Solubility Prediction Method:	http://link.springer.com/article/10.1007/BF02311772
McGowan Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheric.org/files/research/kdb/mol/mol677.mol
KDB:	https://www.cheric.org/files/research/kdb/mol/mol677.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105055&Units=SI

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

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