

Benzene, 2,4-dichloro-1-methyl-

Other names:	1,3-dichloro-4-methylbenzene 2,4-Dichlorotoluene 2,4-dichloro-1-methylbenzene Toluene, 2,4-dichloro-
Inchi:	InChI=1S/C7H6Cl2/c1-5-2-3-6(8)4-7(5)9/h2-4H,1H3
InchiKey:	FUNUTBJJKQIVSY-UHFFFAOYSA-N
Formula:	C7H6Cl2
SMILES:	Cc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	161.03
CAS:	95-73-8

Physical Properties

Property code	Value	Unit	Source
gf	77.35	kJ/mol	Joback Method
hf	-5.70	kJ/mol	Joback Method
hfus	15.54	kJ/mol	Joback Method
hvap	43.55	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.302		Crippen Method
mcvol	110.210	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
rinpol	187.00		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	187.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1100.00		NIST Webbook
tb	473.20	K	NIST Webbook
tc	700.48	K	Joback Method
tf	279.95	K	Joback Method
vc	0.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.67	J/molxK	471.06	Joback Method
cpg	195.96	J/molxK	509.30	Joback Method
cpg	204.68	J/molxK	547.53	Joback Method
cpg	212.85	J/molxK	585.77	Joback Method
cpg	220.49	J/molxK	624.01	Joback Method
cpg	227.64	J/molxK	662.24	Joback Method
cpg	234.30	J/molxK	700.48	Joback Method
dvisc	0.0016666	Paxs	279.95	Joback Method
dvisc	0.0010588	Paxs	311.80	Joback Method
dvisc	0.0007317	Paxs	343.65	Joback Method
dvisc	0.0005384	Paxs	375.50	Joback Method
dvisc	0.0004156	Paxs	407.36	Joback Method
dvisc	0.0003331	Paxs	439.21	Joback Method
dvisc	0.0002751	Paxs	471.06	Joback Method
hvapt	50.60	kJ/mol	410.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.40105e+01
Coeff. B	-3.75881e+03
Coeff. C	-7.29910e+01
Temperature range (K), min.	346.90
Temperature range (K), max.	505.09

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	7.15091e+01
Coeff. B	-8.62029e+03
Coeff. C	-8.01181e+00
Coeff. D	2.87786e-06

Temperature range (K), min.	259.65
Temperature range (K), max.	705.00

Datasets

Mass density, kg/m³

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m ³ - Liquid
263.15	97.86	1280.746
263.15	1123.89	1281.41
263.15	2150.08	1282.078
263.15	3971.85	1283.256
263.15	6167.48	1284.655
263.15	7898.48	1285.752
263.15	9974.67	1287.058
273.15	101.87	1270.262
273.15	1168.70	1270.98
273.15	2038.48	1271.569
273.15	4184.12	1273.017
273.15	5901.85	1274.166
273.15	7916.96	1275.502
273.15	10080.10	1276.917
273.15	11859.30	1278.072
273.15	14023.90	1279.464
273.15	16108.40	1280.788
273.15	17842.30	1281.881
273.15	20076.00	1283.276
273.15	22131.90	1284.547
273.15	24150.50	1285.785
273.15	26075.70	1286.947
273.15	27912.80	1288.061
273.15	29994.00	1289.3
293.15	97.54	1249.314
293.16	1126.71	1250.082
293.17	1886.78	1250.652
293.18	4191.90	1252.359
293.19	6062.35	1253.73
293.20	7970.06	1255.113
293.21	10164.90	1256.679

293.22	12144.00	1258.087
293.23	14100.90	1259.459
293.24	16101.30	1260.848
293.25	18109.90	1262.226
293.26	20077.20	1263.554
293.27	22135.50	1264.942
293.28	24103.40	1266.25
293.29	25961.70	1267.476
293.30	27896.30	1268.742
293.31	29828.60	1269.998
313.15	107.85	1228.386
313.15	1095.73	1229.211
313.15	2082.65	1230.022
313.15	4107.17	1231.674
313.15	5854.63	1233.08
313.15	8123.14	1234.888
313.15	10162.50	1236.487
313.15	12123.50	1238.006
313.15	13892.20	1239.361
313.15	16106.50	1241.042
313.15	18086.10	1242.52
313.15	20143.90	1244.041
313.15	22019.90	1245.416
313.15	24013.70	1246.859
313.15	25938.10	1248.234
313.15	27775.80	1249.538
313.15	29827.60	1250.978
333.15	101.71	1207.383
333.15	1081.65	1208.275
333.15	1877.77	1208.998
333.15	3933.05	1210.851
333.15	5993.05	1212.681
333.15	8164.28	1214.583
333.15	10140.50	1216.287
333.15	12129.10	1217.977
333.15	14157.30	1219.677
333.15	16128.60	1221.308
333.15	18148.40	1222.96
333.15	20045.80	1224.49
333.15	22094.00	1226.119
333.15	24025.80	1227.64
333.15	25826.10	1229.042
333.15	27856.30	1230.606
333.15	29702.40	1232.007

353.15	101.05	1186.204
353.15	1223.95	1187.34
353.15	2054.23	1188.178
353.15	4178.04	1190.3
353.15	6020.58	1192.109
353.15	8131.50	1194.145
353.15	10112.60	1196.024
353.15	12081.40	1197.868
353.15	14117.60	1199.739
353.15	16085.30	1201.527
353.15	18057.70	1203.289
353.15	19979.70	1204.984
353.15	22046.30	1206.781
353.15	24055.60	1208.502
353.15	26024.80	1210.171
353.15	27872.20	1211.714
353.15	29803.80	1213.316
373.15	99.43	1164.779
373.15	1084.40	1165.894
373.15	1956.51	1166.871
373.15	4135.41	1169.289
373.15	5954.62	1171.267
373.15	7981.30	1173.428
373.15	10128.00	1175.674
373.15	11936.00	1177.539
373.15	14002.50	1179.625
373.15	15987.40	1181.598
373.15	18115.70	1183.682
373.15	19989.90	1185.498
373.15	22002.00	1187.396
373.15	23973.40	1189.24
373.15	26011.40	1191.114
373.15	28050.40	1192.964
373.15	29921.50	1194.643
393.15	100.49	1143.033
393.15	1179.48	1144.396
393.15	1991.45	1145.418
393.15	3926.62	1147.803
393.15	5963.77	1150.268
393.15	7963.70	1152.638
393.15	10152.50	1155.171
393.15	12148.50	1157.433
393.15	14137.40	1159.653
393.15	16116.40	1161.814

393.15	17916.80	1163.747
393.15	20141.00	1166.094
393.15	22095.50	1168.12
393.15	24174.00	1170.233
393.15	26159.60	1172.224
393.15	27968.10	1174.003
393.15	29926.90	1175.919
413.15	100.59	1120.918
413.15	1151.63	1122.413
413.15	2145.34	1123.811
413.15	3981.28	1126.345
413.15	6146.60	1129.268
413.15	8164.11	1131.917
413.15	10060.20	1134.353
413.15	11926.60	1136.701
413.15	14144.60	1139.432
413.15	16149.80	1141.844
413.15	18124.30	1144.175
413.15	20124.50	1146.49
413.15	22138.70	1148.774
413.15	24073.10	1150.924
413.15	26090.80	1153.131
413.15	29979.10	1157.28
433.15	95.11	1098.158
433.15	1136.65	1099.852
433.15	2147.69	1101.453
433.15	3917.76	1104.21
433.15	6150.53	1107.594
433.15	8148.51	1110.531
433.15	10046.10	1113.259
433.15	12142.10	1116.175
433.15	14150.60	1118.907
433.15	16186.80	1121.618
433.15	18165.40	1124.186
433.15	20168.20	1126.732
433.15	22137.80	1129.181
433.15	24092.90	1131.563
433.15	26057.00	1133.915
433.15	28002.60	1136.199
433.15	29939.20	1138.435
453.15	1198.47	1076.81
453.15	2151.66	1078.53
453.15	4164.40	1082.075
453.15	6169.55	1085.471

453.15	8024.43	1088.532
453.15	10086.40	1091.847
453.15	12118.80	1094.988
453.15	14143.90	1098.053
453.15	16087.30	1100.887
453.15	19984.20	1106.47
453.15	22044.30	1109.28
453.15	24087.40	1112.012
453.15	26125.00	1114.677
453.15	28000.40	1117.083
453.15	29897.20	1119.486
473.15	1132.46	1052.656
473.15	2054.35	1054.566
473.15	4181.88	1058.813
473.15	5970.87	1062.272
473.15	8153.54	1066.335
473.15	10137.90	1069.908
473.15	12108.70	1073.331
473.15	14124.60	1073.331
473.15	16133.40	1080.012
473.15	18132.30	1083.191
473.15	20146.90	1086.297
473.15	22083.30	1089.222
473.15	24078.50	1092.15
473.15	26042.80	1094.963
473.15	27886.30	1097.55
473.15	29892.60	1100.313

Reference

<https://www.doi.org/10.1016/j.jct.2008.02.020>

Sources

Measurement and correlation of the (p, T) relation of liquid n-heptane, n-hexane, 2,4-dichlorotoluene, and bromobenzene in the temperature range from (233.15 to 473.15) K at pressures up to 30 MPa for use as reference liquids.	https://www.doi.org/10.1016/j.jct.2008.02.020
Crippen Method:	https://www.thermopedia.com/doc/thermophys/kdb/mol/mol1697.mol
Joback Method:	https://www.thermopedia.com/doc/thermophys/kdb/hcprop/showprop.php?cmpid=1697
NIST Webbook:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
McGowan Method:	https://en.wikipedia.org/wiki/Joback_method
	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95738&Units=SI
	https://www.chemeo.com/doc/models/crippen_log10ws
	https://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	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
rho:	Liquid Density
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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