

Benzene, propyl-

Other names:	1-PHENYLPROPANE 1-Propylbenzene Benzene, n-propyl- ISOCUMENE NSC 16941 Phenylpropane Propylbenzene UN 2364 n-Propylbenzene
Inchi:	InChI=1S/C9H12/c1-2-6-9-7-4-3-5-8-9/h3-5,7-8H,2,6H2,1H3
InchiKey:	ODLMAHJVESYWTB-UHFFFAOYSA-N
Formula:	C9H12
SMILES:	CCCC1CCCCC1
Mol. weight [g/mol]:	120.19
CAS:	103-65-1

Physical Properties

Property code	Value	Unit	Source
af	0.3440		KDB
affp	790.10	kJ/mol	NIST Webbook
basg	762.40	kJ/mol	NIST Webbook
chl	-5214.80	kJ/mol	NIST Webbook
chl	-5218.24 ± 0.67	kJ/mol	NIST Webbook
gf	137.30	kJ/mol	KDB
hcg	5218.24	kJ/mol	KDB
hcn	4954.149	kJ/mol	KDB
hf	7.82 ± 0.84	kJ/mol	NIST Webbook
hf	7.83	kJ/mol	KDB
hfl	-38.40 ± 0.84	kJ/mol	NIST Webbook
hfus	13.11	kJ/mol	Joback Method
hvap	46.24	kJ/mol	NIST Webbook
hvap	46.20	kJ/mol	NIST Webbook
hvap	46.10 ± 2.10	kJ/mol	NIST Webbook
hvap	46.20	kJ/mol	NIST Webbook
hvap	46.22	kJ/mol	NIST Webbook
hvap	45.00	kJ/mol	NIST Webbook
hvap	46.20	kJ/mol	NIST Webbook

hvap	46.20	kJ/mol	NIST Webbook
ie	8.71	eV	NIST Webbook
ie	8.77 ± 0.08	eV	NIST Webbook
ie	8.71	eV	NIST Webbook
ie	8.72 ± 0.01	eV	NIST Webbook
ie	8.71 ± 0.01	eV	NIST Webbook
ie	8.72 ± 0.01	eV	NIST Webbook
log10ws	-3.37		Aqueous Solubility Prediction Method
log10ws	-3.37		Estimated Solubility Method
logp	2.639		Crippen Method
mcvol	113.910	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
pc	3200.00 ± 6.00	kPa	NIST Webbook
pc	3170.00 ± 4.90	kPa	NIST Webbook
pc	3200.00	kPa	KDB
pc	3200.00 ± 10.00	kPa	NIST Webbook
rhoc	272.83 ± 1.20	kg/m3	NIST Webbook
rhoc	272.71 ± 3.61	kg/m3	NIST Webbook
rinpol	938.14		NIST Webbook
rinpol	943.90		NIST Webbook
rinpol	964.60		NIST Webbook
rinpol	973.00		NIST Webbook
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ripol	1213.00		NIST Webbook
ripol	1188.00		NIST Webbook
ripol	1207.00		NIST Webbook
sg	397.86	J/mol×K	NIST Webbook
sl	287.78	J/mol×K	NIST Webbook
tb	432.39	K	KDB
tc	638.35	K	KDB
tc	638.80 ± 0.60	K	NIST Webbook
tc	639.20 ± 0.40	K	NIST Webbook
tc	638.36 ± 0.30	K	NIST Webbook
tc	638.24 ± 0.10	K	NIST Webbook
tc	638.40 ± 0.10	K	NIST Webbook
tf	171.60 ± 0.25	K	NIST Webbook
tf	171.64 ± 0.30	K	NIST Webbook
tf	171.28 ± 0.40	K	NIST Webbook
tf	173.58 ± 0.20	K	NIST Webbook
tf	173.56 ± 0.02	K	NIST Webbook
tf	173.40 ± 0.40	K	NIST Webbook
tf	173.69 ± 0.20	K	NIST Webbook

tf	171.60 ± 0.04	K	NIST Webbook
tf	173.57 ± 0.04	K	NIST Webbook
tf	173.59 ± 0.03	K	NIST Webbook
tf	173.65 ± 0.02	K	NIST Webbook
tf	173.06 ± 0.40	K	NIST Webbook
tf	174.00 ± 0.60	K	NIST Webbook
tf	173.08 ± 0.10	K	NIST Webbook
tf	173.59	K	KDB
tf	173.53	K	Aqueous Solubility Prediction Method
tf	174.10	K	Phase equilibria of didecyldimethylammonium nitrate ionic liquid with water and organic solvents
tf	171.50 ± 0.20	K	NIST Webbook
tf	173.95 ± 0.30	K	NIST Webbook
tt	173.59 ± 0.01	K	NIST Webbook
tt	171.60 ± 0.01	K	NIST Webbook
vc	0.440	m3/kmol	KDB
vc	0.440	m3/kmol	NIST Webbook
zc	0.2652820		KDB
zra	0.26		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.49	J/mol×K	604.58	Joback Method
cpg	228.81	J/mol×K	466.52	Joback Method
cpg	266.38	J/mol×K	570.06	Joback Method
cpg	254.59	J/mol×K	535.55	Joback Method
cpg	242.07	J/mol×K	501.03	Joback Method
cpg	287.94	J/mol×K	639.09	Joback Method
cpg	214.76	J/mol×K	432.00	Joback Method
cpl	214.72	J/mol×K	298.15	NIST Webbook
cpl	184.00	J/mol×K	295.00	NIST Webbook
dvisc	0.0016197	Pa×s	253.34	Joback Method
dvisc	0.0004002	Pa×s	360.54	Joback Method
dvisc	0.0002971	Pa×s	396.27	Joback Method
dvisc	0.0005756	Pa×s	324.81	Joback Method
dvisc	0.0009057	Pa×s	289.07	Joback Method
dvisc	0.0002317	Pa×s	432.00	Joback Method
dvisc	0.0035055	Pa×s	217.61	Joback Method

hfust	9.27	kJ/mol	173.60	NIST Webbook
hfust	9.27	kJ/mol	173.60	NIST Webbook
hvapt	38.24	kJ/mol	430.20	KDB
hvapt	43.80	kJ/mol	365.50	NIST Webbook
hvapt	42.70	kJ/mol	390.50	NIST Webbook
rfi	1.49150		293.10	Extraction of propylbenzene or butylbenzene from dodecane using 4-methyl-N-butylpyridinium tetrafluoroborate, [mebupy][BF ₄], as an ionic liquid at different temperatures
rfi	1.48951		298.15	KDB
rfi	1.49010		298.15	Liquid-Liquid(-Liquid) Equilibria in Ternary Systems of Water + Cyclohexylamine + Aromatic Hydrocarbon (Toluene or Propylbenzene) or Aliphatic Hydrocarbon (Heptane or Octane)
rfi	1.48580		303.15	Densities, Viscosities, and Refractive Indices of Binary Mixtures of Anisole with Benzene, Methylbenzene, Ethylbenzene, Propylbenzene, and Butylbenzene at (293.15 and 303.15) K
rfi	1.49150		293.10	Liquid liquid equilibria for n-alkanes (C ₁₂ , C ₁₄ , C ₁₇) + propylbenzene +NMP mixtures at temperatures between 298 and 328K
rfi	1.49150		293.10	Evaluation of [bmim][PF ₆] as an ionic solvent for the extraction of propylbenzene from aliphatic compounds

rfi	1.49160		293.15	Densities, Viscosities, and Refractive Indices of Binary Mixtures of Anisole with Benzene, Methylbenzene, Ethylbenzene, Propylbenzene, and Butylbenzene at (293.15 and 303.15) K
rhoI	857.62	kg/m3	298.15	Excess Enthalpies of Chloroalkylbenzene + Alkylbenzene Mixtures
rhoI	840.90	kg/m3	318.15	The density, the refractive index and the adjustment of the excess thermodynamic properties by means of the multiple linear regression method for the ternary system ethylbenzene-octane-propylbenzene
rhoI	849.40	kg/m3	308.15	The density, the refractive index and the adjustment of the excess thermodynamic properties by means of the multiple linear regression method for the ternary system ethylbenzene-octane-propylbenzene
rhoI	857.90	kg/m3	298.15	The density, the refractive index and the adjustment of the excess thermodynamic properties by means of the multiple linear regression method for the ternary system ethylbenzene-octane-propylbenzene

rhoI	837.31	kg/m3	323.15	Densities, speeds of sound, refractive indices, viscosities and their related thermodynamic properties for n-hexadecane + two aromatic hydrocarbons binary mixtures at temperatures from 298.15 K to 318.15 K
rhoI	845.81	kg/m3	313.15	Densities, speeds of sound, refractive indices, viscosities and their related thermodynamic properties for n-hexadecane + two aromatic hydrocarbons binary mixtures at temperatures from 298.15 K to 318.15 K
rhoI	854.28	kg/m3	303.15	Densities, speeds of sound, refractive indices, viscosities and their related thermodynamic properties for n-hexadecane + two aromatic hydrocarbons binary mixtures at temperatures from 298.15 K to 318.15 K
rhoI	862.72	kg/m3	293.15	Densities, speeds of sound, refractive indices, viscosities and their related thermodynamic properties for n-hexadecane + two aromatic hydrocarbons binary mixtures at temperatures from 298.15 K to 318.15 K

rhoI	850.01	kg/m3	308.15	Densities, speeds of sound, refractive indices, viscosities and their related thermodynamic properties for n-hexadecane + two aromatic hydrocarbons binary mixtures at temperatures from 298.15 K to 318.15 K
rhoI	858.62	kg/m3	298.15	Phase behaviour of ionic liquid 1-butyl-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate with alcohols, water and aromatic hydrocarbons
rhoI	857.62	kg/m3	298.15	Thermodynamic study of 1,1,2,2-tetrachloroethane + hydrocarbon mixtures I. Excess and solvation enthalpies
rhoI	862.00	kg/m3	293.00	KDB
rhoI	858.45	kg/m3	298.15	Densities, speeds of sound, refractive indices, viscosities and their related thermodynamic properties for n-hexadecane + two aromatic hydrocarbons binary mixtures at temperatures from 298.15 K to 318.15 K
rhoI	841.53	kg/m3	318.15	Densities, speeds of sound, refractive indices, viscosities and their related thermodynamic properties for n-hexadecane + two aromatic hydrocarbons binary mixtures at temperatures from 298.15 K to 318.15 K
srf	0.03	N/m	293.20	KDB

tcondl	0.12	W/m×K	329.54	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	329.79	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	312.97	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	312.79	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	312.54	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.13	W/m×K	294.60	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	294.42	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	294.17	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	275.33	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	275.09	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.14	W/m×K	261.57	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.14	W/m×K	261.40	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.14	W/m×K	261.18	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	329.98	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	275.50	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.45214e+01
Coeff. B	-3.81126e+03
Coeff. C	-4.75350e+01
Temperature range (K), min.	315.30
Temperature range (K), max.	461.35

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	8.95794e+01
Coeff. B	-8.51249e+03
Coeff. C	-1.09449e+01
Coeff. D	6.16532e-06
Temperature range (K), min.	173.67
Temperature range (K), max.	638.38

Sources

A 1-alkylcyclopentadienylpyridinium-based ionic liquid in the separation processes: (Solid + liquid) and (liquid + liquid) phase equilibria study and correlation thermodynamic systems and Thermal diffusivity of ethylbutylamine liquid + hexadecane system (1998) 1044, 1045, 1046, 1047, 1048, 1049, 1050, 1051, 1052, 1053, 1054, 1055, 1056, 1057, 1058, 1059, 1060, 1061, 1062, 1063, 1064, 1065, 1066, 1067, 1068, 1069, 1070, 1071, 1072, 1073, 1074, 1075, 1076, 1077, 1078, 1079, 1080, 1081, 1082, 1083, 1084, 1085, 1086, 1087, 1088, 1089, 1090, 1091, 1092, 1093, 1094, 1095, 1096, 1097, 1098, 1099, 1100, 1101, 1102, 1103, 1104, 1105, 1106, 1107, 1108, 1109, 1110, 1111, 1112, 1113, 1114, 1115, 1116, 1117, 1118, 1119, 1120, 1121, 1122, 1123, 1124, 1125, 1126, 1127, 1128, 1129, 1130, 1131, 1132, 1133, 1134, 1135, 1136, 1137, 1138, 1139, 1140, 1141, 1142, 1143, 1144, 1145, 1146, 1147, 1148, 1149, 1150, 1151, 1152, 1153, 1154, 1155, 1156, 1157, 1158, 1159, 1160, 1161, 1162, 1163, 1164, 1165, 1166, 1167, 1168, 1169, 1170, 1171, 1172, 1173, 1174, 1175, 1176, 1177, 1178, 1179, 1180, 1181, 1182, 1183, 1184, 1185, 1186, 1187, 1188, 1189, 1190, 1191, 1192, 1193, 1194, 1195, 1196, 1197, 1198, 1199, 1200, 1201, 1202, 1203, 1204, 1205, 1206, 1207, 1208, 1209, 1210, 1211, 1212, 1213, 1214, 1215, 1216, 1217, 1218, 1219, 1220, 1221, 1222, 1223, 1224, 1225, 1226, 1227, 1228, 1229, 1230, 1231, 1232, 1233, 1234, 1235, 1236, 1237, 1238, 1239, 1240, 1241, 1242, 1243, 1244, 1245, 1246, 1247, 1248, 1249, 1250, 1251, 1252, 1253, 1254, 1255, 1256, 1257, 1258, 1259, 1260, 1261, 1262, 1263, 1264, 1265, 1266, 1267, 1268, 1269, 1270, 1271, 1272, 1273, 1274, 1275, 1276, 1277, 1278, 1279, 1280, 1281, 1282, 1283, 1284, 1285, 1286, 1287, 1288, 1289, 1290, 1291, 1292, 1293, 1294, 1295, 1296, 1297, 1298, 1299, 1300, 1301, 1302, 1303, 1304, 1305, 1306, 1307, 1308, 1309, 1310, 1311, 1312, 1313, 1314, 1315, 1316, 1317, 1318, 1319, 1320, 1321, 1322, 1323, 1324, 1325, 1326, 1327, 1328, 1329, 1330, 1331, 1332, 1333, 1334, 1335, 1336, 1337, 1338, 1339, 1340, 1341, 1342, 1343, 1344, 1345, 1346, 1347, 1348, 1349, 1350, 1351, 1352, 1353, 1354, 1355, 1356, 1357, 1358, 1359, 1360, 1361, 1362, 1363, 1364, 1365, 1366, 1367, 1368, 1369, 1370, 1371, 1372, 1373, 1374, 1375, 1376, 1377, 1378, 1379, 1380, 1381, 1382, 1383, 1384, 1385, 1386, 1387, 1388, 1389, 1390, 1391, 1392, 1393, 1394, 1395, 1396, 1397, 1398, 1399, 1400, 1401, 1402, 1403, 1404, 1405, 1406, 1407, 1408, 1409, 1410, 1411, 1412, 1413, 1414, 1415, 1416, 1417, 1418, 1419, 1420, 1421, 1422, 1423, 1424, 1425, 1426, 1427, 1428, 1429, 1430, 1431, 1432, 1433, 1434, 1435, 1436, 1437, 1438, 1439, 1440, 1441, 1442, 1443, 1444, 1445, 1446, 1447, 1448, 1449, 1450, 1451, 1452, 1453, 1454, 1455, 1456, 1457, 1458, 1459, 1460, 1461, 1462, 1463, 1464, 1465, 1466, 1467, 1468, 1469, 1470, 1471, 1472, 1473, 1474, 1475, 1476, 1477, 1478, 1479, 1480, 1481, 1482, 1483, 1484, 1485, 1486, 1487, 1488, 1489, 1490, 1491, 1492, 1493, 1494, 1495, 1496, 1497, 1498, 1499, 1500, 1501, 1502, 1503, 1504, 1505, 1506, 1507, 1508, 1509, 1510, 1511, 1512, 1513, 1514, 1515, 1516, 1517, 1518, 1519, 1520, 1521, 1522, 1523, 1524, 1525, 1526, 1527, 1528, 1529, 1530, 1531, 1532, 1533, 1534, 1535, 1536, 1537, 1538, 1539, 1540, 1541, 1542, 1543, 1544, 1545, 1546, 1547, 1548, 1549, 1550, 1551, 1552, 1553, 1554, 1555, 1556, 1557, 1558, 1559, 1560, 1561, 1562, 1563, 1564, 1565, 1566, 1567, 1568, 1569, 1570, 1571, 1572, 1573, 1574, 1575, 1576, 1577, 1578, 1579, 1580, 1581, 1582, 1583, 1584, 1585, 1586, 1587, 1588, 1589, 1590, 1591, 1592, 1593, 1594, 1595, 1596, 1597, 1598, 1599, 1600, 1601, 1602, 1603, 1604, 1605, 1606, 1607, 1608, 1609, 1610, 1611, 1612, 1613, 1614, 1615, 1616, 1617, 1618, 1619, 1620, 1621, 1622, 1623, 1624, 1625, 1626, 1627, 1628, 1629, 1630, 1631, 1632, 1633, 1634, 1635, 1636, 1637, 1638, 1639, 1640, 1641, 1642, 1643, 1644, 1645, 1646, 1647, 1648, 1649, 1650, 1651, 1652, 1653, 1654, 1655, 1656, 1657, 1658, 1659, 1660, 1661, 1662, 1663, 1664, 1665, 1666, 1667, 1668, 1669, 1670, 1671, 1672, 1673, 1674, 1675, 1676, 1677, 1678, 1679, 1680, 1681, 1682, 1683, 1684, 1685, 1686, 1687, 1688, 1689, 1690, 1691, 1692, 1693, 1694, 1695, 1696, 1697, 1698, 1699, 1700, 1701, 1702, 1703, 1704, 1705, 1706, 1707, 1708, 1709, 1710, 1711, 1712, 1713, 1714,

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Phase equilibria of didecyldimethylammonium nitrate ionic liquid with trialkylamines and organic solvents: Chloroalkylbenzene + Alkylbenzene Activity coefficients at infinite dilution

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C103651&Units=SI>

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hcg:	Heat of Combustion, Gross form
hcn:	Heat of Combustion, Net Form
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
rhoc:	Critical density
rho:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sg:	Molar entropy at standard conditions
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter

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