

Tris(2,2,2-trinitroethyl)orthoformate

Inchi: InChI=1S/C7H7N9O21/c17-8(18)5(9(19)20,10(21)22)1-35-4(36-2-6(11(23)24,12(25)26)13-7-3)/q17-19,21-23,25-27,29-31,33-35,37-39,41-43,45-47,49-51,53-55,57-59,61-63,65-67,69-71,73-75,77-79,81-83,85-87,89-91,93-95,97-99,101-103,105-107,109-111,113-115,117-119,121-123,125-127,129-131,133-135,137-139,141-143,145-147,149-151,153-155,157-159,161-163,165-167,169-171,173-175,177-179,181-183,185-187,189-191,193-195,197-199,201-203,205-207,209-211,213-215,217-219,221-223,225-227,229-231,233-235,237-239,241-243,245-247,249-251,253-255,257-259,261-263,265-267,269-271,273-275,277-279,281-283,285-287,289-291,293-295,297-299,301-303,305-307,309-311,313-315,317-319,321-323,325-327,329-331,333-335,337-339,341-343,345-347,349-351,353-355,357-359,361-363,365-367,369-371,373-375,377-379,381-383,385-387,389-391,393-395,397-399,401-403,405-407,409-411,413-415,417-419,421-423,425-427,429-431,433-435,437-439,441-443,445-447,449-451,453-455,457-459,461-463,465-467,469-471,473-475,477-479,481-483,485-487,489-491,493-495,497-499,501-503,505-507,509-511,513-515,517-519,521-523,525-527,529-531,533-535,537-539,541-543,545-547,549-551,553-555,557-559,561-563,565-567,569-571,573-575,577-579,581-583,585-587,589-591,593-595,597-599,601-603,605-607,609-611,613-615,617-619,621-623,625-627,629-631,633-635,637-639,641-643,645-647,649-651,653-655,657-659,661-663,665-667,669-671,673-675,677-679,681-683,685-687,689-691,693-695,697-699,701-703,705-707,709-711,713-715,717-719,721-723,725-727,729-731,733-735,737-739,741-743,745-747,749-751,753-755,757-759,761-763,765-767,769-771,773-775,777-779,781-783,785-787,789-791,793-795,797-799,801-803,805-807,809-811,813-815,817-819,821-823,825-827,829-831,833-835,837-839,841-843,845-847,849-851,853-855,857-859,861-863,865-867,869-871,873-875,877-879,881-883,885-887,889-891,893-895,897-899,901-903,905-907,909-911,913-915,917-919,921-923,925-927,929-931,933-935,937-939,941-943,945-947,949-951,953-955,957-959,961-963,965-967,969-971,973-975,977-979,981-983,985-987,989-991,993-995,997-999,1001-1003,1005-1007,1009-1011,1013-1015,1017-1019,1021-1023,1025-1027,1029-1031,1033-1035,1037-1039,1041-1043,1045-1047,1049-1051,1053-1055,1057-1059,1061-1063,1065-1067,1069-1071,1073-1075,1077-1079,1081-1083,1085-1087,1089-1091,1093-1095,1097-1099,1101-1103,1105-1107,1109-1111,1113-1115,1117-1119,1121-1123,1125-1127,1129-1131,1133-1135,1137-1139,1141-1143,1145-1147,1149-1151,1153-1155,1157-1159,1161-1163,1165-1167,1169-1171,1173-1175,1177-1179,1181-1183,1185-1187,1189-1191,1193-1195,1197-1199,1201-1203,1205-1207,1209-1211,1213-1215,1217-1219,1221-1223,1225-1227,1229-1231,1233-1235,1237-1239,1241-1243,1245-1247,1249-1251,1253-1255,1257-1259,1261-1263,1265-1267,1269-1271,1273-1275,1277-1279,1281-1283,1285-1287,1289-1291,1293-1295,1297-1299,1301-1303,1305-1307,1309-1311,1313-1315,1317-1319,1321-1323,1325-1327,1329-1331,1333-1335,1337-1339,1341-1343,1345-1347,1349-1351,1353-1355,1357-1359,1361-1363,1365-1367,1369-1371,1373-1375,1377-1379,1381-1383,1385-1387,1389-1391,1393-1395,1397-1399,1401-1403,1405-1407,1409-1411,1413-1415,1417-1419,1421-1423,1425-1427,1429-1431,1433-1435,1437-1439,1441-1443,1445-1447,1449-1451,1453-1455,1457-1459,1461-1463,1465-1467,1469-1471,1473-1475,1477-1479,1481-1483,1485-1487,1489-1491,1493-1495,1497-1499,1501-1503,1505-1507,1509-1511,1513-1515,1517-1519,1521-1523,1525-1527,1529-1531,1533-1535,1537-1539,1541-1543,1545-1547,1549-1551,1553-1555,1557-1559,1561-1563,1565-1567,1569-1571,1573-1575,1577-1579,1581-1583,1585-1587,1589-1591,1593-1595,1597-1599,1601-1603,1605-1607,1609-1611,1613-1615,1617-1619,1621-1623,1625-1627,1629-1631,1633-1635,1637-1639,1641-1643,1645-1647,1649-1651,1653-1655,1657-1659,1661-1663,1665-1667,1669-1671,1673-1675,1677-1679,1681-1683,1685-1687,1689-1691,1693-1695,1697-1699,1701-1703,1705-1707,1709-1711,1713-1715,1717-1719,1721-1723,1725-1727,1729-1731,1733-1735,1737-1739,1741-1743,1745-1747,1749-1751,1753-1755,1757-1759,1761-1763,1765-1767,1769-1771,1773-1775,1777-1779,1781-1783,1785-1787,1789-1791,1793-1795,1797-1799,1801-1803,1805-1807,1809-1811,1813-1815,1817-1819,1821-1823,1825-1827,1829-1831,1833-1835,1837-1839,1841-1843,1845-1847,1849-1851,1853-1855,1857-1859,1861-1863,1865-1867,1869-1871,1873-1875,1877-1879,1881-1883,1885-1887,1889-1891,1893-1895,1897-1899,1901-1903,1905-1907,1909-1911,1913-1915,1917-1919,1921-1923,1925-1927,1929-1931,1933-1935,1937-1939,1941-1943,1945-1947,1949-1951,1953-1955,1957-1959,1961-1963,1965-1967,1969-1971,1973-1975,1977-1979,1981-1983,1985-1987,1989-1991,1993-1995,1997-1999,2001-2003,2005-2007,2009-2011,2013-2015,2017-2019,2021-2023,2025-2027,2029-2031,2033-2035,2037-2039,2041-2043,2045-2047,2049-2051,2053-2055,2057-2059,2061-2063,2065-2067,2069-2071,2073-2075,2077-2079,2081-2083,2085-2087,2089-2091,2093-2095,2097-2099,2101-2103,2105-2107,2109-2111,2113-2115,2117-2119,2121-2123,2125-2127,2129-2131,2133-2135,2137-2139,2141-2143,2145-2147,2149-2151,2153-2155,2157-2159,2161-2163,2165-2167,2169-2171,2173-2175,2177-2179,2181-2183,2185-2187,2189-2191,2193-2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Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14548595&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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