

# Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, gamma-lactone, triacetate

InChI: InChI=1S/C13H16O8/c1-6(14)18-9-4-13(21-8(3)16)5-10(20-12(13)17)11(9)19-7(2)15/h9-13,21-22,24-25,27-28,30-31,33-34,36-37,39-40,42-43,45-46,48-49,51-52,54-55,57-58,60-61,63-64,66-67,69-70,72-73,75-76,78-79,81-82,84-85,87-88,90-91,93-94,96-97,99-100,102-103,105-106,108-109,111-112,114-115,117-118,120-121,123-124,126-127,129-130,132-133,135-136,138-139,141-142,144-145,147-148,150-151,153-154,156-157,159-160,162-163,165-166,168-169,171-172,174-175,177-178,180-181,183-184,186-187,189-190,192-193,195-196,198-199,201-202,204-205,207-208,210-211,213-214,216-217,219-220,222-223,225-226,228-229,231-232,234-235,237-238,240-241,243-244,246-247,249-250,252-253,255-256,258-259,261-262,264-265,267-268,270-271,273-274,276-277,279-280,282-283,285-286,288-289,291-292,294-295,297-298,300-301,303-304,306-307,309-310,312-313,315-316,318-319,321-322,324-325,327-328,330-331,333-334,336-337,339-340,342-343,345-346,348-349,351-352,354-355,357-358,360-361,363-364,366-367,369-370,372-373,375-376,378-379,381-382,384-385,387-388,390-391,393-394,396-397,399-400,402-403,405-406,408-409,411-412,414-415,417-418,420-421,423-424,426-427,429-430,432-433,435-436,438-439,441-442,444-445,447-448,450-451,453-454,456-457,459-460,462-463,465-466,468-469,471-472,474-475,477-478,480-481,483-484,486-487,489-490,492-493,495-496,498-499,501-502,504-505,507-508,510-511,513-514,516-517,519-520,522-523,525-526,528-529,531-532,534-535,537-538,540-541,543-544,546-547,549-550,552-553,555-556,558-559,561-562,564-565,567-568,570-571,573-574,576-577,579-580,582-583,585-586,588-589,591-592,594-595,597-598,599-600,602-603,605-606,608-609,611-612,614-615,617-618,620-621,623-624,626-627,629-630,632-633,635-636,638-639,641-642,644-645,647-648,650-651,653-654,656-657,659-660,662-663,665-666,668-669,671-672,674-675,677-678,680-681,683-684,686-687,689-690,692-693,695-696,698-699,701-702,704-705,707-708,710-711,713-714,716-717,719-720,722-723,725-726,728-729,731-732,734-735,737-738,740-741,743-744,746-747,749-750,752-753,755-756,758-759,761-762,764-765,767-768,770-771,773-774,776-777,779-780,782-783,785-786,788-789,791-792,794-795,797-798,799-800,802-803,805-806,808-809,811-812,814-815,817-818,819-820,822-823,825-826,828-829,831-832,834-835,837-838,840-841,843-844,845-846,848-849,851-852,854-855,857-858,859-860,862-863,865-866,868-869,871-872,874-875,877-878,879-880,882-883,885-886,888-889,891-892,894-895,897-898,899-900,902-903,905-906,908-909,911-912,914-915,917-918,919-920,922-923,925-926,928-929,931-932,934-935,937-938,939-940,942-943,945-946,948-949,951-952,954-955,957-958,959-960,962-963,965-966,968-969,971-972,974-975,977-978,979-980,982-983,985-986,988-989,991-992,994-995,997-998,999-1000,1002-1003,1005-1006,1008-1009,1011-1012,1014-1015,1017-1018,1019-1020,1022-1023,1025-1026,1028-1029,1031-1032,1034-1035,1037-1038,1039-1040,1042-1043,1045-1046,1048-1049,1051-1052,1054-1055,1057-1058,1059-1060,1062-1063,1065-1066,1068-1069,1071-1072,1074-1075,1077-1078,1079-1080,1082-1083,1085-1086,1088-1089,1091-1092,1094-1095,1097-1098,1099-1100,1102-1103,1105-1106,1108-1109,1111-1112,1114-1115,1117-1118,1119-1120,1122-1123,1125-1126,1128-1129,1131-1132,1134-1135,1137-1138,1139-1140,1142-1143,1145-1146,1148-1149,1151-1152,1154-1155,1157-1158,1159-1160,1162-1163,1165-1166,1168-1169,1171-1172,1174-1175,1177-1178,1179-1180,1182-1183,1185-1186,1188-1189,1191-1192,1194-1195,1197-1198,1199-1200,1202-1203,1205-1206,1208-1209,1211-1212,1214-1215,1217-1218,1219-1220,1222-1223,1225-1226,1228-1229,1231-1232,1234-1235,1237-1238,1239-1240,1242-1243,1245-1246,1248-1249,1251-1252,1254-1255,1257-1258,1259-1260,1262-1263,1265-1266,1268-1269,1271-1272,1274-1275,1277-1278,1279-1280,1282-1283,1285-1286,1288-1289,1291-1292,1294-1295,1297-1298,1299-1300,1302-1303,1305-1306,1308-1309,1311-1312,1314-1315,1317-1318,1319-1320,1322-1323,1325-1326,1328-1329,1331-1332,1334-1335,1337-1338,1339-1340,1342-1343,1345-1346,1348-1349,1351-1352,1354-1355,1357-1358,1359-1360,1362-1363,1365-1366,1368-1369,1371-1372,1374-1375,1377-1378,1379-1380,1382-1383,1385-1386,1388-1389,1391-1392,1394-1395,1397-1398,1399-1400,1402-1403,1405-1406,1408-1409,1411-1412,1414-1415,1417-1418,1419-1420,1422-1423,1425-1426,1428-1429,1431-1432,1434-1435,1437-1438,1439-1440,1442-1443,1445-1446,1448-1449,1451-1452,1454-1455,1457-1458,1459-1460,1462-1463,1465-1466,1468-1469,1471-1472,1474-1475,1477-1478,1479-1480,1482-1483,1485-1486,1488-1489,1491-1492,1494-1495,1497-1498,1499-1500,1502-1503,1505-1506,1508-1509,1511-1512,1514-1515,1517-1518,1519-1520,1522-1523,1525-1526,1528-1529,1531-1532,1534-1535,1537-1538,1539-1540,1542-1543,1545-1546,1548-1549,1551-1552,1554-1555,1557-1558,1559-1560,1562-1563,1565-1566,1568-1569,1571-1572,1574-1575,1577-1578,1579-1580,1582-1583,1585-1586,1588-1589,1591-1592,1594-1595,1597-1598,1599-1600,1602-1603,1605-1606,1608-1609,1611-1612,1614-1615,1617-1618,1619-1620,1622-1623,1625-1626,1628-1629,1631-1632,1634-1635,1637-1638,1639-1640,1642-1643,1645-1646,1648-1649,1651-1652,1654-1655,1657-1658,1659-1660,1662-1663,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# Sources

|                        |                                                                                                                                               |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                         |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C97101003&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C97101003&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                     |

## Legend

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

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