

I-Serine, N,O-bis(caproyl)-, methyl ester

Inchi: InChI=1S/C16H29NO5/c1-4-6-8-10-14(18)17-13(16(20)21-3)12-22-15(19)11-9-7-5-2/h13-15,17-22,24-25,27-28,30-31,33-34,36-37,39-40,42-43,45-46,48-49,51-52,54-55,57-58,60-61,63-64,66-67,69-70,72-73,75-76,78-79,81-82,84-85,87-88,90-91,93-94,96-97,99-100,102-103,105-106,108-109,111-112,114-115,117-118,120-121,123-124,126-127,129-130,132-133,135-136,138-139,141-142,144-145,147-148,150-151,153-154,156-157,159-160,162-163,165-166,168-169,171-172,174-175,177-178,180-181,183-184,186-187,189-190,192-193,195-196,198-199,201-202,204-205,207-208,210-211,213-214,216-217,219-220,222-223,225-226,228-229,231-232,234-235,237-238,240-241,243-244,246-247,249-250,252-253,255-256,258-259,261-262,264-265,267-268,270-271,273-274,276-277,279-280,282-283,285-286,288-289,291-292,294-295,297-298,300-301,303-304,306-307,309-310,312-313,315-316,318-319,321-322,324-325,327-328,330-331,333-334,336-337,339-340,342-343,345-346,348-349,351-352,354-355,357-358,360-361,363-364,366-367,369-370,372-373,375-376,378-379,381-382,384-385,387-388,390-391,393-394,396-397,399-400,402-403,405-406,408-409,411-412,414-415,417-418,420-421,423-424,426-427,429-430,432-433,435-436,438-439,441-442,444-445,447-448,450-451,453-454,456-457,459-460,462-463,465-466,468-469,471-472,474-475,477-478,480-481,483-484,486-487,489-490,492-493,495-496,498-499,501-502,504-505,507-508,510-511,513-514,516-517,519-520,522-523,525-526,528-529,531-532,534-535,537-538,540-541,543-544,546-547,549-550,552-553,555-556,558-559,561-562,564-565,567-568,569,571-572,574-575,577-578,580-581,583-584,586-587,589-590,592-593,595-596,598-599,601-602,604-605,607-608,610-611,613-614,616-617,619-620,622-623,625-626,628-629,631-632,634-635,637-638,640-641,643-644,646-647,649-650,652-653,655-656,658-659,661-662,664-665,667-668,669,671-672,674-675,677-678,680-681,683-684,686-687,689-690,692-693,695-696,698-699,701-702,704-705,707-708,710-711,713-714,716-717,719-720,722-723,725-726,728-729,731-732,734-735,737-738,740-741,743-744,746-747,749-750,752-753,755-756,758-759,761-762,764-765,767-768,769,771-772,774-775,777-778,780-781,783-784,786-787,789-790,792-793,795-796,798-799,801-802,804-805,807-808,810-811,813-814,816-817,819-820,822-823,825-826,828-829,831-832,834-835,837-838,840-841,843-844,846-847,849-850,852-853,855-856,858-859,861-862,864-865,867-868,869,871-872,874-875,877-878,880-881,883-884,886-887,889-890,892-893,895-896,898-899,901-902,904-905,907-908,910-911,913-914,916-917,919-920,922-923,925-926,928-929,931-932,934-935,937-938,940-941,943-944,946-947,949-950,952-953,955-956,958-959,961-962,964-965,967-968,969,971-972,974-975,977-978,980-981,983-984,986-987,989-990,992-993,995-996,998-999,1001-1002,1004-1005,1007-1008,1010-1011,1013-1014,1016-1017,1019-1020,1022-1023,1025-1026,1028-1029,1031-1032,1034-1035,1037-1038,1040-1041,1043-1044,1046-1047,1049-1050,1052-1053,1055-1056,1058-1059,1061-1062,1064-1065,1067-1068,1069,1071-1072,1074-1075,1077-1078,1080-1081,1083-1084,1086-1087,1089-1090,1092-1093,1095-1096,1098-1099,1101-1102,1104-1105,1107-1108,1110-1111,1113-1114,1116-1117,1119-1120,1122-1123,1125-1126,1128-1129,1131-1132,1134-1135,1137-1138,1140-1141,1143-1144,1146-1147,1149-1150,1152-1153,1155-1156,1158-1159,1161-1162,1164-1165,1167-1168,1169,1171-1172,1174-1175,1177-1178,1180-1181,1183-1184,1186-1187,1189-1190,1192-1193,1195-1196,1198-1199,1201-1202,1204-1205,1207-1208,1210-1211,1213-1214,1216-1217,1219-1220,1222-1223,1225-1226,1228-1229,1231-1232,1234-1235,1237-1238,1240-1241,1243-1244,1246-1247,1249-1250,1252-1253,1255-1256,1258-1259,1261-1262,1264-1265,1267-1268,1269,1271-1272,1274-1275,1277-1278,1280-1281,1283-1284,1286-1287,1289-1290,1292-1293,1295-1296,1298-1299,1301-1302,1304-1305,1307-1308,1310-1311,1313-1314,1316-1317,1319-1320,1322-1323,1325-1326,1328-1329,1331-1332,1334-1335,1337-1338,1340-1341,1343-1344,1346-1347,1349-1350,1352-1353,1355-1356,1358-1359,1361-1362,1364-1365,1367-1368,1369,1371-1372,1374-1375,1377-1378,1380-1381,1383-1384,1386-1387,1389-1390,1392-1393,1395-1396,1398-1399,1401-1402,1404-1405,1407-1408,1410-1411,1413-1414,1416-1417,1419-1420,1422-1423,1425-1426,1428-1429,1431-1432,1434-1435,1437-1438,1440-1441,1443-1444,1446-1447,1449-1450,1452-1453,1455-1456,1458-1459,1461-1462,1464-1465,1467-1468,1469,1471-1472,1474-1475,1477-1478,1480-1481,1483-1484,1486-1487,1489-1490,1492-1493,1495-1496,1498-1499,1501-1502,1504-1505,1507-1508,1510-1511,1513-1514,1516-1517,1519-1520,1522-1523,1525-1526,1528-1529,1531-1532,1534-1535,1537-1538,1540-1541,1543-1544,1546-1547,1549-1550,1552-1553,1555-1556,1558-1559,1561-1562,1564-1565,1567-1568,1569,1571-1572,1574-1575,1577-1578,1580-1581,1583-1584,1586-1587,1589-1590,1592-1593,1595-1596,1598-1599,1601-1602,1604-1605,1607-1608,1610-1611,1613-1614,1616-1617,1619-1620,1622-1623,1625-1626,1628-1629,1631-1632,1634-1635,1637-1638,1640-1641,1643-1644,1646-1647,1649-1650,1652-1653,1655-1656,1658-1659,1661-1662,1664-1665,1667-1668,1669,1671-1672,1674-1675,1677-1678,1680-1681,1683-1684,1686-1687,1689-1690,1692-1693,1695-1696,1698-1699,1701-1702,1704-1705,1707-1708,1710-1711,1713-1714,1716-1717,1719-1720,1722-1723,1725-1726,1728-1729,1731-1732,1734-1735,1737-1738,1740-1741,1743-1744,1746-1747,1749-1750,1752-1753,1755-1756,1758-1759,1761-1762,1764-1765,1767-1768,1769,1771-1772,1774-1775,1777-1778,1780-1781,1783-1784,1786-1787,1789-1790,1792-1793,1795-1796,1798-1799,1801-1802,1804-1805,1807-1808,1810-1811,1813-1814,1816-1817,1819-1820,1822-1823,1825-1826,1828-1829,1831-1832,1834-1835,1837-1838,1840-1841,1843-1844,1846-1847,1849-1850,1852-1853,1855-1856,1858-1859,1861-1862,1864-1865,1867-1868,1869,1871-1872,1874-1875,1877-1878,1880-1881,1883-1884,1886-1887,1889-1890,1892-1893,1895-1896,1898-1899,1901-1902,1904-1905,1907-1908,1910-1911,1913-1914,1916-1917,1919-1920,1922-1923,1925-1926,1928-1929,1931-1932,1934-1935,1937-1938,1940-1941,1943-1944,1946-1947,1949-1950,1952-1953,1955-1956,1958-1959,1961-1962,1964-1965,1967-1968,1969,1971-1972,1974-1975,1977-1978,1980-1981,1983-1984,1986-1987,1989-1990,1992-1993,1995-1996,1998-1999,2001-2002,2004-2005,2007-2008,2010-2011,2013-2014,2016-2017,2019-2020,2022-2023,2025-2026,2028-2029,2031-2032,2034-2035,2037-2038,2040-2041,2043-2044,2046-2047,2049-2050,2052-2053,2055-2056,2058-2059,2061-2062,2064-2065,2067-2068,2069,2071-2072,2074-2075,2077-2078,2080-2081,2083-2084,2086-2087,2089-2090,2092-2093,2095-2096,2098-2099,2101-2102,2104-2105,2107-2108,2110-2111,2113-2114,2116-2117,2119-2120,2122-2123,2125-2126,2128-2129,2131-2132,2134-2135,2137-2138,2140-2141,2143-2144,2146-2147,2149-2150,2152-2153,2155-2156,2158-2159,2161-2162,2164-2165,2167-2168,2169,2171-2172,2174-2175,2177-2178,2180-2181,2183-2184,2186-2187,2189-2190,2192-2193,2195-2196,2198-2199,2201-2202,2204-2205,2207-2208,2210-2211,2213-2214,2216-2217,2219-2220,2222-2223,2225-2226,2228-2229,2231-2232,2234-2235,2237-2238,2240-2241,2243-2244,2246-2247,2249-2250,2252-2253,2255-2256,2258-2259,2261-2262,2264-2265,2267-2268,2269,2271-2272,2274-2275,2277-2278,2280-2281,2283-2284,2286-2287,2289-2290,2292-2293,2295-2296,2298-2299,2301-2302,2304-2305,2307-2308,2310-2311,2313-2314,2316-2317,2319-2320,2322-2323,2325-2326,2328-2329,2331-2332,2334-2335,2337-2338,2340-2341,2343-2344,2346-2347,2349-2350,2352-2353,2355-2356,2358-2359,2361-2362,2364-2365,2367-2368,2369,2371-2372,2374-2375,2377-2378,2380-2381,2383-2384,2386-2387,2389-2390,2392-2393,2395-2396,2398-2399,2401-2402,2404-2405,2407-2408,2410-2411,2413-2414,2416-2417,2419-2420,2422-2423,2425-2426,2428-2429,2431-2432,2434-2435,2437-2438,2440-2441,2443-2444,2446-2447,2449-2450,2452-2453,2455-2456,2458-2459,2461-2462,2464-2465,2467-2468,2469,2471-2472,2474-2475,2477-2478,2480-2481,2483-2484,2486-2487,2489-2490,2492-2493,2495-2496,2498-2499,2501-2502,2504-2505,2507-2508,2510-2511,2513-2514,2516-2517,2519-2520,2522-2523,2525-2526,2528-2529,2531-2532,2534-2535,2537-2538,2540-2541,2543-2544,2546-2547,2549-2550,2552-2553,2555-2556,2558-2559,2561-2562,2564-2565,2567-2568,2569,2571-2572,2574-2575,2577-2578,2580-2581,2583-2584,2586-2587,2589-2590,2592-2593,2595-2596,2598-2599,2601-2602,2604-2605,2607-2608,2610-2611,2613-2614,2616-2617,2619-2620,2622-2623,2625-2626,2628-2629,2631-2632,2634-2635,2637-2638,2640-2641,2643-2644,2646-2647,2649-2650,2652-2653,2655-2656,2658-2659,2661-2662,2664-2665,2667-2668,2669,2671-2672,2674-2675,2677-2678,2680-2681,2683-2684,2686-2687,2689-2690,2692-2693,2695-2696,2698-2699,2701-2702,2704-2705,2707-2708,2710-2711,2713-2714,2716-2717,2719-2720,2722-2723,2725-2726,2728-2729,2731-2732,2734-2735,2737-2738,2740-2741,2743-2744,2746-2747,2749-2750,2752-2753,2755-2756,2758-2759,2761-2762,2764-2765,2767-2768,2769,2771-2772,2774-2775,2777-2778,2780-2781,2783-2784,2786-2787,2789-2790,2792-2793,2795-2796,2798-2799,2801-2802,2804-2805,2807-2808,2810-2811,2813-2814,2816-2817,2819-2820,2822-2823,2825-2826,2828-2829,2831-2832,2834-2835,2837-2838,2840-2841,2843-2844,2846-2847,2849-2850,2852-2853,2855-2856,2858-2859,2861-2862,2864-2865,2867-2868,2869,2871-2872,2874-2875,2877-2878,2880-2881,2883-2884,2886-2887,2889-2890,2892-2893,2895-2896,2898-2899,2901-2902,2904-2905,2907-2908,2910-2911,2913-2914,2916-2917,2919-2920,2922-2923,2925-2926,2928-2929,2931-2932,2934-2935,2937-2938,2940-2941,2943-2944,2946-2947,2949-2950,2952-2953,2955-2956,2958-2959,2961-2962,2964-2965,2967-2968,2969,2971-2972,2974-2975,2977-2978,2980-2981,2983-2984,2986-2987,2989-2990,2992-2993,2995-2996,2998-2999,3001-3002,3004-3005,3007-3008,3010-3011,3013-3014,3016-3017,3019-3020,3022-3023,3025-3026,3028-3029,3031-3032,3034-3035,3037-3038,3040-3041,3043-3044,3046-3047,3049-3050,3052-3053,3055-3056,3058-3059,3061-3062,3064-3065,3067-3068,3069,3071-3072,3074-3075,3077-3078,3080-3081,3083-3084,3086-3087,3089-3090,3092-3093,3095-3096,3098-3099,3101-3102,3104-3105,3107-3108,3110-3111,3113-3114,3116-3117,3119-3120,3122-3123,3125-3126,3128-3129,3131-3132,3134-3135,3137-3138,3140-3141,3143-3144,3146-3147,3149-3150,3152-3153,3155-3156,3158-3159,3161-3162,3164-3165,3167-3168,3169,3171-3172,3174-3175,3177-3178,3180-3181,3183-3184,3186-3187,3189-3190,3192-3193,3195-3196,3198-3199,3201-3202,3204-3205,3207-3208,3210-3211,3213-3214,3216-3217,3219-3220,3222-3223,3225-3226,3228-3229,3231-3232,3234-3235,3237-3238,3240-3241,3243-3244,3246-3247,3249-3250,3252-3253,3255-3256,3258-3259,3261-3262,3264-3265,3267-3268,3269,3271-3272,3274-3275,3277-3278,3280-3281,3283-3284,3286-3287,3289-3290,3292-3293,3295-3296,3298-3299,3301-3302,3304-3305,3307-3308,3310-3311,3313-3314,3316-3317,3319-3320,3322-3323,3325-3326,3328-3329,3331-3332,3334-3335,3337-3338,3340-3341,3343-3344,3346-3347,3349-3350,3352-3353,3355-3356,3358-3359,3361-3362,3364-3365,3367-3368,3369,3371-3372,3374-3375,3377-3378,3380-3381,3383-3384,3386-3387,3389-3390,3392-3393,3395-3396,3398-3399,3401-3402,3404-3405,3407-3408,3410-3411,3413-3414,3416-3417,3419-3420,3422-3423,3425-3426,3428-3429,3431-3432,3434-3435,3437-3438,3440-3441,3443-3444,3446-3447,3449-3450,3452-3453,3455-3456,3458-3459,3461-3462,3464-3465,3467-3468,3469,3471-3472,3474-3475,3477-3478,3480-3481,3483-3484,3486-3487,3489-3490,3492-3493,3495-3496,3498-3499,3501-3502,3504-3505,3507-3508,3510-3511,3513-3514,3516-3517,3519-3520,3522-3523,3525-3526,3528-3529,3531-3532,3534-3535,3537-3538,3540-3541,3543-3544,3546-3547,3549-3550,3552-3553,3555-3556,3558-3559,3561-3562,3564-3565,3567-3568,3569,3571-3572,3574-3575,3577-3578,3580-3581,3583-3584,3586-3587,3589-3590,3592-3593,3595-3596,3598-3599,3601-3602,3604-3605,3607-3608,3610-3611,3613-3614,3616-3617,3619-3620,3622-3623,3625-3626,3628-3629,3631-3632,3634-3635,3637-3638,3640-3641,3643-3644,3646-3647,3649-3650,3652-3653,3655-3656,3658-3659,3661-3662,3664-3665,3667-3668,3669,3671-3672,3674-3675,3677-3678,3680-3681,3683-3684,3686-3687,3689-3690,3692-3693,3695-3696,3698-3699,3701-3702,3704-3705,3707-3708,3710-3711,3713-3714,3716-3717,3719-3720,3722-3723,3725-3726,3728-3729,3731-3732,3734-3735,3737-3738,3740-3741,3743-3744,3746-3747,3749-3750,3752-3753,3755-3756,3758-3759,3761-3762,3764-3765,3767-3768,3769,3771-3772,3774-3775,3777-3778,3780-3781,3783-3784,3786-3787,3789-3790,3792-3793,3795-3796,3798-3799,3801-3802,3804-3805,3807-3808,3810-3811,3813-3814,3816-3817,3819-3820,3822-3823,3825-3826,3828-3829,3831-3832,3834-3835,3837-3838,3840-3841,3843-3844,3846-3847,3849-3850,3852-3853,3855-3856,3858-3859,3861-3862,3864-3865,3867-3868,3869,3871-3872,3874-3875,3877-3878,3880-3881,3

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299738&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

Legend

cpg:	Ideal gas heat capacity
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/46-305-2/l-Serine-N-O-bis-caproyl-methyl-ester.pdf>

Generated by Cheméo on 2025-12-06 03:45:20.955020345 +0000 UTC m=+4740918.485060999.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.