

Succinic acid, hex-4-yn-3-yl 1-bromo-3,3,3-trifluoroprop-2-yl ester

Inchi: InChI=1S/C13H16BrF3O4/c1-3-5-9(4-2)20-11(18)6-7-12(19)21-10(8-14)13(15,16)17/h9-12,20-21,23-24,26-27,29-30,32-33,35-36,38-39,41-42,44-45,47-48,50-51,53-54,56-57,59-60,62-63,65-66,68-69,71-72,74-75,77-78,80-81,83-84,86-87,89-90,92-93,95-96,98-99,101-102,104-105,107-108,110-111,113-114,116-117,119-120,122-123,125-126,128-129,131-132,134-135,137-138,140-141,143-144,146-147,149-150,152-153,155-156,158-159,161-162,164-165,167-168,170-171,173-174,176-177,179-180,182-183,185-186,188-189,191-192,194-195,197-198,200-201,203-204,206-207,209-210,212-213,215-216,218-219,221-222,224-225,227-228,230-231,233-234,236-237,239-240,242-243,245-246,248-249,251-252,254-255,257-258,260-261,263-264,266-267,269-270,272-273,275-276,278-279,281-282,284-285,287-288,290-291,293-294,296-297,299-300,302-303,305-306,308-309,311-312,314-315,317-318,320-321,323-324,326-327,329-330,332-333,335-336,338-339,341-342,344-345,347-348,350-351,353-354,356-357,359-360,362-363,365-366,368-369,371-372,374-375,377-378,380-381,383-384,386-387,389-390,392-393,395-396,398-399,401-402,404-405,407-408,410-411,413-414,416-417,419-420,422-423,425-426,428-429,431-432,434-435,437-438,440-441,443-444,446-447,449-450,452-453,455-456,458-459,461-462,464-465,467-468,470-471,473-474,476-477,479-480,482-483,485-486,488-489,491-492,494-495,497-498,499-500,501-502,503-504,505-506,507-508,509-510,511-512,513-514,515-516,517-518,519-520,521-522,523-524,525-526,527-528,529-530,531-532,533-534,535-536,537-538,539-540,541-542,543-544,545-546,547-548,549-550,551-552,553-554,555-556,557-558,559-560,561-562,563-564,565-566,567-568,569-570,571-572,573-574,575-576,577-578,579-580,581-582,583-584,585-586,587-588,589-590,591-592,593-594,595-596,597-598,599-600,601-602,603-604,605-606,607-608,609-610,611-612,613-614,615-616,617-618,619-620,621-622,623-624,625-626,627-628,629-630,631-632,633-634,635-636,637-638,639-640,641-642,643-644,645-646,647-648,649-650,651-652,653-654,655-656,657-658,659-660,661-662,663-664,665-666,667-668,669-670,671-672,673-674,675-676,677-678,679-680,681-682,683-684,685-686,687-688,689-690,691-692,693-694,695-696,697-698,699-700,701-702,703-704,705-706,707-708,709-710,711-712,713-714,715-716,717-718,719-720,721-722,723-724,725-726,727-728,729-730,731-732,733-734,735-736,737-738,739-740,741-742,743-744,745-746,747-748,749-750,751-752,753-754,755-756,757-758,759-760,761-762,763-764,765-766,767-768,769-770,771-772,773-774,775-776,777-778,779-780,781-782,783-784,785-786,787-788,789-790,791-792,793-794,795-796,797-798,799-800,801-802,803-804,805-806,807-808,809-810,811-812,813-814,815-816,817-818,819-820,821-822,823-824,825-826,827-828,829-830,831-832,833-834,835-836,837-838,839-840,841-842,843-844,845-846,847-848,849-850,851-852,853-854,855-856,857-858,859-860,861-862,863-864,865-866,867-868,869-870,871-872,873-874,875-876,877-878,879-880,881-882,883-884,885-886,887-888,889-890,891-892,893-894,895-896,897-898,899-900,901-902,903-904,905-906,907-908,909-910,911-912,913-914,915-916,917-918,919-920,921-922,923-924,925-926,927-928,929-930,931-932,933-934,935-936,937-938,939-940,941-942,943-944,945-946,947-948,949-950,951-952,953-954,955-956,957-958,959-960,961-962,963-964,965-966,967-968,969-970,971-972,973-974,975-976,977-978,979-980,981-982,983-984,985-986,987-988,989-990,991-992,993-994,995-996,997-998,999-1000,1001-1002,1003-1004,1005-1006,1007-1008,1009-1010,1011-1012,1013-1014,1015-1016,1017-1018,1019-1020,1021-1022,1023-1024,1025-1026,1027-1028,1029-1030,1031-1032,1033-1034,1035-1036,1037-1038,1039-1040,1041-1042,1043-1044,1045-1046,1047-1048,1049-1050,1051-1052,1053-1054,1055-1056,1057-1058,1059-1060,1061-1062,1063-1064,1065-1066,1067-1068,1069-1070,1071-1072,1073-1074,1075-1076,1077-1078,1079-1080,1081-1082,1083-1084,1085-1086,1087-1088,1089-1090,1091-1092,1093-1094,1095-1096,1097-1098,1099-1100,1101-1102,1103-1104,1105-1106,1107-1108,1109-1110,1111-1112,1113-1114,1115-1116,1117-1118,1119-1120,1121-1122,1123-1124,1125-1126,1127-1128,1129-1130,1131-1132,1133-1134,1135-1136,1137-1138,1139-1140,1141-1142,1143-1144,1145-1146,1147-1148,1149-1150,1151-1152,1153-1154,1155-1156,1157-1158,1159-1160,1161-1162,1163-1164,1165-1166,1167-1168,1169-1170,1171-1172,1173-1174,1175-1176,1177-1178,1179-1180,1181-1182,1183-1184,1185-1186,1187-1188,1189-1190,1191-1192,1193-1194,1195-1196,1197-1198,1199-1200,1201-1202,1203-1204,1205-1206,1207-1208,1209-1210,1211-1212,1213-1214,1215-1216,1217-1218,1219-1220,1221-1222,1223-1224,1225-1226,1227-1228,1229-1230,1231-1232,1233-1234,1235-1236,1237-1238,1239-1240,1241-1242,1243-1244,1245-1246,1247-1248,1249-1250,1251-1252,1253-1254,1255-1256,1257-1258,1259-1260,1261-1262,1263-1264,1265-1266,1267-1268,1269-1270,1271-1272,1273-1274,1275-1276,1277-1278,1279-1280,1281-1282,1283-1284,1285-1286,1287-1288,1289-1290,1291-1292,1293-1294,1295-1296,1297-1298,1299-1300,1301-1302,1303-1304,1305-1306,1307-1308,1309-1310,1311-1312,1313-1314,1315-1316,1317-1318,1319-1320,1321-1322,1323-1324,1325-1326,1327-1328,1329-1330,1331-1332,1333-1334,1335-1336,13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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

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