

1-Deoxy-1-(methylamino)-D-galactitol, N,O,O,O,O,O-hexa(trifluoroacetyl)-

Inchi: InChI=1S/C19H11F18NO11/c1-38(8(39)14(20,21)22)2-4(46-10(41)16(26,27)28)6(48-12(49)18)11(50)13(51)15(52)17(53)19(54)55(56)57(58)59(60)61(62)63(64)65(66)67(68)69(70)71(72)73(74)75(76)77(78)79(80)81(82)83(84)85(86)87(88)89(90)91(92)93(94)95(96)97(98)99(100)101(102)103(104)105(106)107(108)109(110)111(112)113(114)115(116)117(118)119(120)121(122)123(124)125(126)127(128)129(130)131(132)133(134)135(136)137(138)139(140)141(142)143(144)145(146)147(148)149(150)151(152)153(154)155(156)157(158)159(160)161(162)163(164)165(166)167(168)169(170)171(172)173(174)175(176)177(178)179(180)181(182)183(184)185(186)187(188)189(190)191(192)193(194)195(196)197(198)199(200)201(202)203(204)205(206)207(208)209(210)211(212)213(214)215(216)217(218)219(220)221(222)223(224)225(226)227(228)229(230)231(232)233(234)235(236)237(238)239(240)241(242)243(244)245(246)247(248)249(250)251(252)253(254)255(256)257(258)259(260)261(262)263(264)265(266)267(268)269(270)271(272)273(274)275(276)277(278)279(280)281(282)283(284)285(286)287(288)289(290)291(292)293(294)295(296)297(298)299(300)301(302)303(304)305(306)307(308)309(310)311(312)313(314)315(316)317(318)319(320)321(322)323(324)325(326)327(328)329(330)331(332)333(334)335(336)337(338)339(340)341(342)343(344)345(346)347(348)349(350)351(352)353(354)355(356)357(358)359(360)361(362)363(364)365(366)367(368)369(370)371(372)373(374)375(376)377(378)379(380)381(382)383(384)385(386)387(388)389(390)391(392)393(394)395(396)397(398)399(400)401(402)403(404)405(406)407(408)409(410)411(412)413(414)415(416)417(418)419(420)421(422)423(424)425(426)427(428)429(430)431(432)433(434)435(436)437(438)439(440)441(442)443(444)445(446)447(448)449(450)451(452)453(454)455(456)457(458)459(460)461(462)463(464)465(466)467(468)469(470)471(472)473(474)475(476)477(478)479(480)481(482)483(484)485(486)487(488)489(490)491(492)493(494)495(496)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(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InchiKey: AINUEIDIXPMVIA-UHFFFAOYSA-N

Formula: C19H11F18NO11

SMILES: CN(CC(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(COC(=O)C(F)(F)F)O

Mol. weight [g/mol]: 771.26

Physical Properties

Property code	Value	Unit	Source
gf	-4577.94	kJ/mol	Joback Method
hf	-5308.14	kJ/mol	Joback Method
hfus	60.38	kJ/mol	Joback Method
hvap	88.42	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	3.009		Crippen Method
mvol	359.180	ml/mol	McGowan Method
pc	857.47	kPa	Joback Method
rinpol	1293.50		NIST Webbook
rinpol	1293.50		NIST Webbook
tb	1047.60	K	Joback Method
tc	1351.34	K	Joback Method
tf	712.23	K	Joback Method
vc	1.478	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1211.70	J/molxK	1047.60	Joback Method
cpg	1219.75	J/molxK	1098.22	Joback Method
cpg	1226.27	J/molxK	1148.85	Joback Method
cpg	1231.63	J/molxK	1199.47	Joback Method
cpg	1236.16	J/molxK	1250.09	Joback Method
cpg	1240.23	J/molxK	1300.72	Joback Method
cpg	1244.20	J/molxK	1351.34	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U380295&Units=SI

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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