

Benzene-hexa-n-hexanoate

Inchi:	InChI=1S/C42H66O12/c1-7-13-19-25-31(43)49-37-38(50-32(44)26-20-14-8-2)40(52-34(45)39-35-21-15-9-3)41(53-36(46)42-33-22-16-10-4)44(54-38(47)41-32(48)40-27-17-11-5-1)42(55-39(49)43-34(50)41-32(51)40-27-17-11-5-1)44(56-40(52)42-33-22-16-10-4)46(57-41(53)43-34(54)41-32(55)40-27-17-11-5-1)48(58-43(56)45-36(57)41-32(58)40-27-17-11-5-1)50(59-46(58)48-39(59)41-32(60)40-27-17-11-5-1)52(61-49(60)51-42(61)41-32(62)40-27-17-11-5-1)54(63-52(64)54-47(65)41-32(66)40-27-17-11-5-1)56(67-54(68)56-51(69)41-32(70)40-27-17-11-5-1)58(71-56(72)58-55(73)41-32(74)40-27-17-11-5-1)60(75-58(76)60-57(77)41-32(78)40-27-17-11-5-1)62(79-60(80)62-59(81)41-32(82)40-27-17-11-5-1)64(83-62(84)64-61(85)41-32(86)40-27-17-11-5-1)66(87-64(88)66-63(89)41-32(90)40-27-17-11-5-1)68(91-66(92)68-65(93)41-32(94)40-27-17-11-5-1)70(95-68(96)70-67(97)41-32(98)40-27-17-11-5-1)72(99-70(100)72-69(101)41-32(102)40-27-17-11-5-1)74(103-72(104)74-71(105)41-32(106)40-27-17-11-5-1)76(107-74(108)76-73(109)41-32(110)40-27-17-11-5-1)78(111-76(112)78-75(113)41-32(114)40-27-17-11-5-1)80(115-78(116)80-77(117)41-32(118)40-27-17-11-5-1)82(119-80(120)82-79(121)41-32(122)40-27-17-11-5-1)84(123-82(124)84-81(125)41-32(126)40-27-17-11-5-1)86(127-84(128)86-83(129)41-32(130)40-27-17-11-5-1)88(131-86(132)88-85(133)41-32(134)40-27-17-11-5-1)90(135-88(136)90-87(137)41-32(138)40-27-17-11-5-1)92(139-90(140)92-89(141)41-32(142)40-27-17-11-5-1)94(143-92(144)94-91(145)41-32(146)40-27-17-11-5-1)96(147-94(148)96-93(149)41-32(150)40-27-17-11-5-1)98(151-96(152)98-95(153)41-32(154)40-27-17-11-5-1)100(155-98(156)100-97(157)41-32(158)40-27-17-11-5-1)102(159-100(160)102-99(161)41-32(162)40-27-17-11-5-1)104(163-102(164)104-101(165)41-32(166)40-27-17-11-5-1)106(167-104(168)106-103(169)41-32(170)40-27-17-11-5-1)108(171-106(172)108-105(173)41-32(174)40-27-17-11-5-1)110(175-108(176)110-107(177)41-32(178)40-27-17-11-5-1)112(179-110(180)112-109(181)41-32(182)40-27-17-11-5-1)114(183-112(184)114-111(185)41-32(186)40-27-17-11-5-1)116(187-114(188)116-113(189)41-32(190)40-27-17-11-5-1)118(191-116(192)118-115(193)41-32(194)40-27-17-11-5-1)120(195-118(196)120-117(197)41-32(198)40-27-17-11-5-1)122(199-120(200)122-119(201)41-32(202)40-27-17-11-5-1)124(203-122(204)124-121(205)41-32(206)40-27-17-11-5-1)126(207-124(208)126-123(209)41-32(210)40-27-17-11-5-1)128(211-126(212)128-125(213)41-32(214)40-27-17-11-5-1)130(215-128(216)130-127(217)41-32(218)40-27-17-11-5-1)132(219-130(220)132-129(221)41-32(222)40-27-17-11-5-1)134(223-132(224)134-131(225)41-32(226)40-27-17-11-5-1)136(227-134(228)136-133(229)41-32(230)40-27-17-11-5-1)138(231-136(232)138-135(233)41-32(234)40-27-17-11-5-1)140(235-138(236)140-137(237)41-32(238)40-27-17-11-5-1)142(239-140(240)142-139(241)41-32(242)40-27-17-11-5-1)144(243-142(244)144-141(245)41-32(246)40-27-17-11-5-1)146(247-144(248)146-143(249)41-32(250)40-27-17-11-5-1)148(251-146(252)148-145(253)41-32(254)40-27-17-11-5-1)150(255-148(256)150-147(257)41-32(258)40-27-17-11-5-1)152(259-150(260)152-149(261)41-32(262)40-27-17-11-5-1)154(263-152(264)154-151(265)41-32(266)40-27-17-11-5-1)156(267-154(268)156-153(269)41-32(270)40-27-17-11-5-1)158(271-156(272)158-155(273)41-32(274)40-27-17-11-5-1)160(275-158(276)160-157(277)41-32(278)40-27-17-11-5-1)162(279-160(280)162-159(281)41-32(282)40-27-17-11-5-1)164(283-162(284)164-161(285)41-32(286)40-27-17-11-5-1)166(287-164(288)166-163(289)41-32(290)40-27-17-11-5-1)168(291-166(292)168-165(293)41-32(294)40-27-17-11-5-1)170(295-168(296)170-167(297)41-32(298)40-27-17-11-5-1)172(299-170(300)172-169(301)41-32(302)40-27-17-11-5-1)174(303-172(304)174-171(305)41-32(306)40-27-17-11-5-1)176(307-174(308)176-173(309)41-32(310)40-27-17-11-5-1)178(311-176(312)178-175(313)41-32(314)40-27-17-11-5-1)180(315-178(316)180-177(317)41-32(318)40-27-17-11-5-1)182(319-180(320)182-179(321)41-32(322)40-27-17-11-5-1)184(323-182(324)184-181(325)41-32(326)40-27-17-11-5-1)186(327-184(328)186-183(329)41-32(330)40-27-17-11-5-1)188(331-186(332)188-185(333)41-32(334)40-27-17-11-5-1)190(335-188(336)190-187(337)41-32(338)40-27-17-11-5-1)192(339-190(340)192-189(341)41-32(342)40-27-17-11-5-1)194(343-192(344)194-191(345)41-32(346)40-27-17-11-5-1)196(347-194(348)196-193(349)41-32(350)40-27-17-11-5-1)198(351-196(352)198-195(353)41-32(354)40-27-17-11-5-1)200(355-198(356)200-197(357)41-32(358)40-27-17-11-5-1)202(359-200(360)202-199(361)41-32(362)40-27-17-11-5-1)204(363-202(364)204-201(365)41-32(366)40-27-17-11-5-1)206(367-204(368)206-203(369)41-32(370)40-27-17-11-5-1)208(371-206(372)208-205(373)41-32(374)40-27-17-11-5-1)210(375-208(376)210-207(377)41-32(378)40-27-17-11-5-1)212(379-210(380)212-209(381)41-32(382)40-27-17-11-5-1)214(383-212(384)214-211(385)41-32(386)40-27-17-11-5-1)216(387-214(388)216-213(389)41-32(390)40-27-17-11-5-1)218(391-216(392)218-215(393)41-32(394)40-27-17-11-5-1)220(395-218(396)220-217(397)41-32(398)40-27-17-11-5-1)222(399-220(400)222-219(401)41-32(402)40-27-17-11-5-1)224(403-222(404)224-221(405)41-32(406)40-27-17-11-5-1)226(407-224(408)226-223(409)41-32(410)40-27-17-11-5-1)228(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cpg	-312.40	J/mol×K	2803.24	Joback Method
cps	1300.00	J/mol×K	300.00	NIST Webbook
cps	1294.90	J/mol×K	298.15	NIST Webbook
dvisc	0.0000004	Pa×s	1669.68	Joback Method
dvisc	0.0000027	Pa×s	1085.08	Joback Method
dvisc	0.0000017	Pa×s	1182.51	Joback Method
dvisc	0.0000011	Pa×s	1279.95	Joback Method
dvisc	0.0000008	Pa×s	1377.38	Joback Method
dvisc	0.0000006	Pa×s	1474.81	Joback Method
dvisc	0.0000004	Pa×s	1572.25	Joback Method
hfust	33.50	kJ/mol	203.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65201696&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

tt: Triple Point Temperature
vc: Critical Volume

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