Hexanedioic acid, dipropyl ester

Other names:	Adipic acid di-n-propyl ester
	Di-n-Propyl adipate
	adipic acid, dipropyl ester
	dipropyl adipate
	dipropyl hexanedioate
Inchi:	InChI=1S/C12H22O4/c1-3-9-15-11(13)7-5-6-8-12(14)16-10-4-2/h3-10H2,1-2H3
InchiKey:	NKOUWLLFHNBUDW-UHFFFAOYSA-N
Formula:	C12H22O4
SMILES:	CCCOC(=O)CCCCC(=O)OCCC
Mol. weight [g/mol]:	230.30
CAS:	106-19-4

Physical Properties

Property code	Value	Unit	Source
gf	-417.68	kJ/mol	Joback Method
hf	-780.61	kJ/mol	Joback Method
hfus	32.41	kJ/mol	Joback Method
hvap	60.62	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.453		Crippen Method
mcvol	194.820	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
rinpol	1545.00		NIST Webbook
rinpol	1545.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1588.00		NIST Webbook
rinpol	1544.00		NIST Webbook
rinpol	1545.00		NIST Webbook
rinpol	1554.00		NIST Webbook
rinpol	1544.00		NIST Webbook
rinpol	1569.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1545.00		NIST Webbook
rinpol	1569.00		NIST Webbook
rinpol	1554.00		NIST Webbook
rinpol	1544.00		NIST Webbook
rinpol	1569.00		NIST Webbook

rinpol	1543.00		NIST Webbook
tb	626.54	K	Joback Method
tc	803.91	K	Joback Method
tf	369.32	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.96	J/mol×K	626.54	Joback Method
cpg	593.78	J/mol×K	803.91	Joback Method
cpg	582.39	J/mol×K	774.35	Joback Method
cpg	570.37	J/mol×K	744.79	Joback Method
cpg	557.71	J/mol×K	715.23	Joback Method
cpg	544.42	J/mol×K	685.66	Joback Method
cpg	530.51	J/mol×K	656.10	Joback Method
dvisc	0.0009273	Pa×s	412.19	Joback Method
dvisc	0.0005638	Pa×s	455.06	Joback Method
dvisc	0.0003735	Pa×s	497.93	Joback Method
dvisc	0.0002641	Pa×s	540.80	Joback Method
dvisc	0.0001965	Pa×s	583.67	Joback Method
dvisc	0.0001522	Pa×s	626.54	Joback Method
dvisc	0.0017118	Pa×s	369.32	Joback Method
hvapt	63.60	kJ/mol	476.50	NIST Webbook
pvap	0.05	kPa	361.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.03	kPa	354.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids
pvap	0.03	kPa	351.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids

pvap	0.04	kPa	357.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.02	kPa	348.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.02	kPa	345.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.01	kPa	342.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	9.72e-03	kPa	339.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	7.65e-03	kPa	336.10	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	6.02e-03	kPa	333.20	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	

pvap	3.67e-03	kPa	327.40	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	2.60e-03	kPa	323.50	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	2.22e-03	kPa	321.70	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	0.06	kPa	365.30	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
pvap	1.73e-03	kPa	318.80	Vapor Pressures and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Dicarboxylic Acids	
sdco	0.00	m2/s	338.47	Self-diffusivity measurements of dimethyl, diethyl, dipropyl, dibutyl, Bis(2-ethylhexyl) adipates from (293 - 339) K by a PGSE-NMR spin-echo technique	
sdco	0.00	m2/s	329.45	Self-diffusivity measurements of dimethyl, diethyl, dipropyl, dibutyl, Bis(2-ethylhexyl) adipates from (293 - 339) K by a PGSE-NMR spin-echo technique	

sdco	0.00	m2/s	311.45	Self-diffusivity measurements of dimethyl, diethyl, dipropyl, dibutyl, Bis(2-ethylhexyl) adipates from (293 - 339) K by a PGSE-NMR spin-echo technique
sdco	0.00	m2/s	302.44	Self-diffusivity measurements of dimethyl, diethyl, dipropyl, dibutyl, Bis(2-ethylhexyl) adipates from (293 - 339) K by a PGSE-NMR spin-echo technique
sdco	0.00	m2/s	293.43	Self-diffusivity measurements of dimethyl, diethyl, dipropyl, dibutyl, Bis(2-ethylhexyl) adipates from (293 - 339) K by a PGSE-NMR spin-echo technique
sdco	0.00	m2/s	320.46	Self-diffusivity measurements of dimethyl, diethyl, dipropyl, dibutyl, Bis(2-ethylhexyl) adipates from (293 - 339) K by a PGSE-NMR spin-echo technique

Datasets

Viscosity, Pa*s

Temperature, K - Liquid	Pressure, kPa - Liquid	Viscosity, Pa*s - Liquid
283.15	100.00	0.0061533
283.15	1000.00	0.0062173
283.15	5000.00	0.0065360
283.15	10000.00	0.0069433
283.15	15000.00	0.0073601

283.15	20000.00	0.0078113
283.15	30000.00	0.0087586
283.15	40000.00	0.0097597
293.15	100.00	0.0045992
293.14	1000.00	0.0046501
293.15	5000.00	0.0048701
293.15	10000.00	0.0051548
293.15	15000.00	0.0054559
293.15	20000.00	0.0057726
293.15	30000.00	0.0064294
293.15	40000.00	0.0071687
303.15	100.00	0.0035666
303.15	1000.00	0.0036041
303.15	5000.00	0.0037658
303.15	10000.00	0.0039833
303.15	15000.00	0.0042054
303.15	20000.00	0.0044338
303.15	30000.00	0.0049375
303.15	40000.00	0.0054570
313.15	100.00	0.0028538
313.15	1000.00	0.0028886
313.15	5000.00	0.0030140
313.15	10000.00	0.0031776
313.15	15000.00	0.0033466
313.15	20000.00	0.0035194
313.15	30000.00	0.0038990
313.15	40000.00	0.0042925
323.15	100.00	0.0023397
323.15	1000.00	0.0023637
323.15	5000.00	0.0024644
323.14	10000.00	0.0025920
323.15	15000.00	0.0027247
323.15	20000.00	0.0028674
323.15	30000.00	0.0031569
323.15	40000.00	0.0034745
333.15	100.00	0.0019539
333.15	1000.00	0.0019730
333.15	5000.00	0.0020577
333.15	10000.00	0.0021633
333.15	15000.00	0.0022746
333.15	20000.00	0.0023906
333.15	30000.00	0.0026238
333.15	40000.00	0.0028750
343.15	100.00	0.0016582

343.15	1000.00	0.0016728
343.15	5000.00	0.0017443
343.15	10000.00	0.0018349
343.15	15000.00	0.0019283
343.15	20000.00	0.0020191
343.15	30000.00	0.0022159
343.15	40000.00	0.0024204
353.15	100.00	0.0014259
353.15	1000.00	0.0014399
353.15	5000.00	0.0015003
353.15	10000.00	0.0015771
353.15	15000.00	0.0016539
353.15	20000.00	0.0017357
353.15	30000.00	0.0018997
353.15	40000.00	0.0020742
363.15	100.00	0.0012417
363.15	1000.00	0.0012532
363.15	5000.00	0.0013059
363.15	10000.00	0.0013714
363.15	15000.00	0.0014391
363.15	20000.00	0.0015079
363.15	30000.00	0.0016490
363.15	40000.00	0.0017980

Reference *https://www.doi.org/10.1007/s10765-019-2573-6*

Temperature, K	Pressure, kPa	Viscosity, Pa*s
303.14	1140.00	0.0036090
303.14	1110.00	0.0036060
303.14	1110.00	0.0036070
303.15	2810.00	0.0036530
303.15	2820.00	0.0036570
303.15	2810.00	0.0036540
303.14	5220.00	0.0037810
303.14	5220.00	0.0037760
303.14	5210.00	0.0037800
303.15	10310.00	0.0039750
303.15	10320.00	0.0039720
303.15	10310.00	0.0039750
303.15	15310.00	0.0042180
303.15	15260.00	0.0042130
303.15	15230.00	0.0042180
303.14	18290.00	0.0043300

303.14	18290.00	0.0043310
303.14	18280.00	0.0043270
313.16	1200.00	0.0028820
313.16	1220.00	0.0028820
313.16	1210.00	0.0028790
313.15	2710.00	0.0029340
313.16	2700.00	0.0029330
313.15	2710.00	0.0029310
313.16	5190.00	0.0030160
313.16	5180.00	0.0030100
313.16	5180.00	0.0030100
313.16	10490.00	0.0031770
313.16	10480.00	0.0031760
313.16	10460.00	0.0031780
313.15	15330.00	0.0033540
313.15	15330.00	0.0033560
313.15	15330.00	0.0033580
313.16	18290.00	0.0034450
313.15	18290.00	0.0034410
313.15	18290.00	0.0034430
323.15	1180.00	0.0023600
323.15	1170.00	0.0023560
323.15	1160.00	0.0023590
323.16	2720.00	0.0024120
323.16	2710.00	0.0024090
323.16	2710.00	0.0024080
323.16	5270.00	0.0024620
323.16	5270.00	0.0024620
323.16	5260.00	0.0024640
323.17	10210.00	0.0025980
323.17	10220.00	0.0025970
323.17	10220.00	0.0025970
323.16	15200.00	0.0027310
323.16	15200.00	0.0027310
323.15	15180.00	0.0027290
323.17	18270.00	0.0028120
323.17	18240.00	0.0028140
323.17	18260.00	0.0028160
333.16	1090.00	0.0019750
333.16	1120.00	0.0019790
333.16	1100.00	0.0019790
333.14	2620.00	0.0020090
333.14	2610.00	0.0020060
333.15	2620.00	0.0020090

333.15	5130.00	0.0020520
333.15	5110.00	0.0020500
333.15	5110.00	0.0020520
333.16	10190.00	0.0021650
333.16	10180.00	0.0021630
333.16	10160.00	0.0021670
333.16	15220.00	0.0022730
333.15	15220.00	0.0022730
333.15	15200.00	0.0022740
333.15	18300.00	0.0023430
333.15	18290.00	0.0023380
333.15	18260.00	0.0023390

Reference *https://www.doi.org/10.1016/j.fluid.2015.03.016*

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
293.15	100.00	979.3
293.15	520.00	979.7
293.15	1040.00	980.0
293.15	2530.00	981.0
293.15	5020.00	982.5
293.15	7510.00	984.1
293.15	7530.00	984.2
293.15	10010.00	985.7
293.15	15050.00	988.9
293.15	20010.00	991.8
293.15	30030.00	997.7
293.15	39800.00	1003.1
293.15	50070.00	1008.4
293.15	65000.00	1015.7
303.15	100.00	970.3
303.15	100.00	970.4
303.15	500.00	970.7
303.15	1010.00	971.1
303.15	2510.00	972.1
303.15	2510.00	972.1
303.15	5000.00	973.8
303.15	7510.00	975.5
303.15	10020.00	977.1

303.15	15010.00	980.4
303.15	20000.00	983.5
303.15	30010.00	989.6
303.15	39800.00	995.2
303.15	50010.00	1000.7
303.15	64990.00	1008.3
313.15	100.00	961.5
313.15	500.00	961.8
313.15	1010.00	962.2
313.15	2510.00	963.3
313.15	5040.00	965.1
313.15	7510.00	966.8
313.15	10010.00	968.5
313.15	15000.00	971.9
313.15	19980.00	975.2
313.15	30000.00	981.6
313.15	39810.00	987.4
313.15	39800.00	987.4
313.15	50060.00	993.2
313.15	65000.00	1001.0
323.15	100.00	952.4
323.15	500.00	952.8
323.15	1010.00	953.2
323.15	2530.00	954.3
323.15	5020.00	956.2
323.15	7510.00	958.0
323.15	7550.00	958.1
323.15	10000.00	959.9
323.15	15030.00	963.4
323.15	20010.00	966.9
323.15	30010.00	973.5
323.15	39820.00	979.5
323.15	50020.00	985.5
323.15	64990.00	993.7
333.15	100.00	943.5
333.15	500.00	943.9
333.15	1020.00	944.3
333.15	2520.00	945.5
333.15	5010.00	947.5
333.15	7510.00	949.4
333.15	7510.00	949.4
333.15	10000.00	951.3
333.15	15000.00	955.1
333.15	20000.00	958.7

333.15	30020.00	965.6
333.15	39790.00	971.9
333.15	50050.00	978.1
333.15	65000.00	986.5
343.15	100.00	934.6
343.15	520.00	935.0
343.15	1040.00	935.5
343.15	2540.00	936.7
343.15	5020.00	938.8
343.15	7520.00	940.8
343.15	7510.00	940.8
343.15	10020.00	942.8
343.15	15000.00	946.7
343.15	20030.00	950.6
343.15	29580.00	957.4
343.15	39860.00	964.3
343.15	50020.00	970.7
343.15	65000.00	979.4
353.15	100.00	925.7
353.15	510.00	926.1
353.15	1020.00	926.5
353.15	2530.00	927.9
353.15	5020.00	930.1
353.15	7510.00	932.2
353.15	7530.00	932.2
353.15	10000.00	934.3
353.15	14550.00	938.0
353.15	20020.00	942.3
353.15	30010.00	949.8
353.15	39800.00	956.7
353.15	49990.00	963.4
353.15	64990.00	972.4
363.15	100.00	916.7
363.15	500.00	917.2
363.15	980.00	917.6
363.15	2520.00	919.1
363.15	5000.00	921.3
363.15	7480.00	923.6
363.15	7480.00	923.6
363.15	10020.00	925.8
363.15	15020.00	930.1
363.15	20020.00	934.2
363.15	30020.00	942.0
363.15	39810.00	949.1

363.15	50050.00	956.1
363.15	64970.00	965.4
303.15	100.00	970.4
303.15	510.00	970.7
303.15	5030.00	973.8
303.15	10010.00	977.1
303.15	30000.00	989.6
303.15	65010.00	1008.3

Reference *https://www.doi.org/10.1016/j.fluid.2014.04.018*

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106194&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Viscosity measurements of compressed liquid dipropyl and dibutyl adipates:	https://www.doi.org/10.1016/j.fluid.2015.03.016
Density measurements of compressed dipropyl, dibutyl, bis(2-ethylhexyl) adipates from (293 to 373 K) at pressures up to about 68 MPa:	https://www.doi.org/10.1016/j.fluid.2014.04.018
Vapor Pressure and Enthalpies of Vaporization of a Series of the Symmetric Linear n-Alkyl Esters of Adipic Acid:	https://www.doi.org/10.1021/je100231g
Viscosity Measurements of Dialkyl Adipates in the Temperature Range of (293 to 368) K and up to 40 MPa:	https://www.doi.org/10.1007/s10765-019-2573-6
Self-diffusivity measurements of dimethyl, diethyl, dipropyl, dibutyl, Bis(2-ethylhexyl) adipates from (293 - 339) K by a PGSE-NMR spin-echo technique:	https://www.doi.org/10.1016/j.fluid.2015.11.020

Legend

cpg:	Ideal gas 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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure

rhol:	Liquid Density
rinpol:	Non-polar retention indices
sdco:	Self diffusion coefficient
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume