

Acetic acid, 2-ethylhexyl ester

Other names:	.beta.-ethylhexyl acetate 1-hexanol, 2-ethyl-, acetate 2-ETHYL-1-HEXANOL ACETATE 2-ETHYLHEXYL ACETATE 2-ETHYLHEXYL ETHANOATE 2-Ethyl-1-hexyl acetate 2-Ethylhexanyl acetate 2-Ethylhexylester kyseliny octove Acetic acid «alpha»-ethylhexyl ester Acetic acid Â«alphaÂ»-ethylhexyl ester Ethyl(2)-hexyl acetate NSC 8897 Octyl acetate «beta»-Ethylhexyl acetate Â«betaÂ»-Ethylhexyl acetate
Inchi:	InChI=1S/C10H20O2/c1-4-6-7-10(5-2)8-12-9(3)11/h10H,4-8H2,1-3H3
InchiKey:	WOYWLLHHWAMFCB-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CCCCC(CC)COC(C)=O
Mol. weight [g/mol]:	172.26
CAS:	103-09-3

Physical Properties

Property code	Value	Unit	Source
gf	-203.04	kJ/mol	Joback Method
hf	-499.81	kJ/mol	Joback Method
hfus	20.92	kJ/mol	Joback Method
hvap	46.62	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.766		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=2)		KDB
pc	2216.62	kPa	Joback Method
rinpol	1144.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1144.00		NIST Webbook

rinpol	1159.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1099.00		NIST Webbook
ripol	1420.00		NIST Webbook
ripol	1420.00		NIST Webbook
tb	471.65	K	NIST Webbook
tb	473.00	K	NIST Webbook
tb	472.20	K	NIST Webbook
tc	679.81	K	Joback Method
tf	259.62	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.31	J/mol×K	504.05	Joback Method
cpg	396.77	J/mol×K	562.64	Joback Method
cpg	410.17	J/mol×K	591.93	Joback Method
cpg	423.03	J/mol×K	621.22	Joback Method
cpg	435.35	J/mol×K	650.52	Joback Method
cpg	447.14	J/mol×K	679.81	Joback Method
cpg	382.82	J/mol×K	533.34	Joback Method
dvisc	0.0019627	Pa×s	300.36	Joback Method
dvisc	0.0010151	Pa×s	341.10	Joback Method
dvisc	0.0006043	Pa×s	381.84	Joback Method
dvisc	0.0003976	Pa×s	422.57	Joback Method
dvisc	0.0002816	Pa×s	463.31	Joback Method
dvisc	0.0002109	Pa×s	504.05	Joback Method
dvisc	0.0046674	Pa×s	259.62	Joback Method
hvapt	50.10	kJ/mol	402.50	NIST Webbook
rhoI	810.49	kg/m3	363.15	Surface tension of four oxygenated fuels: experiment and correlation
rhoI	814.98	kg/m3	358.15	Surface tension of four oxygenated fuels: experiment and correlation

rhoI	819.45	kg/m3	353.15	Surface tension of four oxygenated fuels: experiment and correlation
rhoI	823.91	kg/m3	348.15	Surface tension of four oxygenated fuels: experiment and correlation
rhoI	828.35	kg/m3	343.15	Surface tension of four oxygenated fuels: experiment and correlation
rhoI	832.78	kg/m3	338.15	Surface tension of four oxygenated fuels: experiment and correlation
rhoI	837.20	kg/m3	333.15	Surface tension of four oxygenated fuels: experiment and correlation
rhoI	841.61	kg/m3	328.15	Surface tension of four oxygenated fuels: experiment and correlation
rhoI	846.01	kg/m3	323.15	Surface tension of four oxygenated fuels: experiment and correlation
rhoI	850.39	kg/m3	318.15	Surface tension of four oxygenated fuels: experiment and correlation
rhoI	854.77	kg/m3	313.15	Surface tension of four oxygenated fuels: experiment and correlation
rhoI	859.15	kg/m3	308.15	Surface tension of four oxygenated fuels: experiment and correlation
rhoI	863.51	kg/m3	303.15	Surface tension of four oxygenated fuels: experiment and correlation
rhoI	872.25	kg/m3	298.15	Liquid-liquid equilibria of water + acetic acid + 2-ethyl hexyl acetate ternary system

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.53661e+01
Coeff. B	-4.29457e+03
Coeff. C	-7.26220e+01
Temperature range (K), min.	357.44
Temperature range (K), max.	499.75

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	9.61783e+01
Coeff. B	-1.03818e+04
Coeff. C	-1.14383e+01
Coeff. D	3.89320e-06
Temperature range (K), min.	180.15
Temperature range (K), max.	639.00

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
283.46	100.00	880.38
283.46	1000.00	881.05
283.47	3000.00	882.48
283.47	5000.00	883.9
283.48	10000.00	887.37
283.48	15000.00	890.63
283.48	20000.00	893.87
283.48	25000.00	896.91

283.47	30000.00	899.95
283.46	40000.00	905.65
283.46	50000.00	911.06
283.46	60000.00	916.18
283.46	70000.00	921.22
283.45	80000.00	925.84
283.45	90000.00	930.33
283.45	100000.00	934.63
293.46	100.00	871.89
293.44	1000.00	872.61
293.44	3000.00	874.12
293.45	5000.00	875.6
293.45	10000.00	879.24
293.45	15000.00	882.73
293.45	20000.00	886.08
293.45	25000.00	889.32
293.45	30000.00	892.46
293.45	40000.00	898.43
293.46	50000.00	904.07
293.45	60000.00	909.42
293.45	70000.00	914.46
293.45	80000.00	919.33
293.46	90000.00	923.91
293.45	100000.00	928.38
303.41	100.00	862.94
303.38	1000.00	863.7
303.39	3000.00	865.32
303.40	5000.00	866.89
303.40	10000.00	870.7
303.39	15000.00	874.36
303.40	20000.00	877.88
303.40	25000.00	881.31
303.40	30000.00	884.55
303.39	40000.00	890.82
303.40	50000.00	896.67
303.40	60000.00	902.22
303.40	70000.00	907.5
303.40	80000.00	912.5
303.40	90000.00	917.28
303.41	100000.00	921.87
313.34	100.00	854.53
313.34	1000.00	855.28
313.34	3000.00	857.04
313.34	5000.00	858.73

313.34	10000.00	862.77
313.34	15000.00	866.66
313.34	20000.00	870.34
313.34	25000.00	873.92
313.34	30000.00	877.34
313.34	40000.00	883.88
313.34	50000.00	889.98
313.34	60000.00	895.7
313.34	70000.00	901.14
313.34	80000.00	906.27
313.35	90000.00	911.19
313.34	100000.00	915.93
323.15	100.00	845.74
323.16	1000.00	846.56
323.16	3000.00	848.36
323.16	5000.00	850.14
323.16	10000.00	854.42
323.17	15000.00	858.49
323.17	20000.00	862.39
323.16	25000.00	866.13
323.16	30000.00	869.71
323.16	40000.00	876.47
323.15	50000.00	882.8
323.15	60000.00	888.76
323.15	70000.00	894.49
323.15	80000.00	899.83
323.15	90000.00	904.91
323.15	100000.00	909.78
332.99	100.00	836.98
333.00	1000.00	837.85
333.00	3000.00	839.78
333.00	5000.00	841.66
333.00	10000.00	846.16
333.00	15000.00	850.47
333.00	20000.00	854.55
333.00	25000.00	858.45
333.01	30000.00	862.21
333.01	40000.00	869.27
333.01	50000.00	875.85
333.01	60000.00	882.02
333.01	70000.00	888.07
333.01	80000.00	893.58
333.01	90000.00	898.82
333.01	100000.00	903.81

342.95	100.00	828.32
342.96	1000.00	829.27
342.96	3000.00	831.31
342.96	5000.00	833.3
342.96	10000.00	838.06
342.96	15000.00	842.59
342.96	20000.00	846.9
342.97	25000.00	851.0
342.97	30000.00	854.91
342.97	40000.00	862.31
342.97	50000.00	869.15
342.97	60000.00	875.57
342.97	70000.00	881.64
342.97	80000.00	887.28
342.97	90000.00	892.73
342.97	100000.00	897.85
352.78	100.00	819.64
352.79	1000.00	820.65
352.79	3000.00	822.83
352.79	5000.00	824.93
352.79	10000.00	830.0
352.79	15000.00	834.75
352.79	20000.00	839.27
352.79	25000.00	843.56
352.79	30000.00	847.66
352.79	40000.00	855.34
352.79	50000.00	862.46
352.79	60000.00	869.08
352.79	70000.00	875.42
352.80	80000.00	881.29
352.79	90000.00	886.84
352.79	100000.00	892.14
362.64	100.00	810.91
362.64	1000.00	811.97
362.64	3000.00	814.28
362.64	5000.00	816.51
362.64	10000.00	821.85
362.64	15000.00	826.87
362.64	20000.00	831.61
362.64	25000.00	836.09
362.64	30000.00	840.38
362.65	40000.00	848.4
362.64	50000.00	855.78
362.64	60000.00	862.65

362.64	70000.00	869.14
362.64	80000.00	875.25
362.64	90000.00	880.97
362.64	100000.00	886.45

Reference

<https://www.doi.org/10.1021/acs.jced.5b00385>

Thermal conductivity, W/m/K

Temperature, K - Liquid	Pressure, kPa - Liquid	Thermal conductivity, W/m/K - Liquid
236.69	20000.00	0.1443
236.98	100.00	0.1389
237.14	10000.00	0.1415
237.23	5000.00	0.1405
237.83	15000.00	0.1430
237.87	100.00	0.1391
237.89	20000.00	0.1444
237.90	15000.00	0.1431
238.15	100.00	0.1390
238.49	20000.00	0.1438
238.60	5000.00	0.1403
238.64	10000.00	0.1417
238.65	15000.00	0.1429
239.43	5000.00	0.1404
239.50	10000.00	0.1416
255.44	100.00	0.1363
255.58	5000.00	0.1382
255.67	20000.00	0.1420
255.73	5000.00	0.1377
255.73	15000.00	0.1409
256.24	20000.00	0.1423
256.27	15000.00	0.1408
256.36	10000.00	0.1399
256.74	20000.00	0.1420
256.94	15000.00	0.1407
257.05	10000.00	0.1397
257.53	5000.00	0.1376
258.31	100.00	0.1361
258.36	100.00	0.1363
258.36	10000.00	0.1390
275.57	100.00	0.1331

275.68	5000.00	0.1354
276.08	15000.00	0.1377
276.34	10000.00	0.1366
276.56	5000.00	0.1343
276.61	15000.00	0.1372
276.71	20000.00	0.1393
276.82	10000.00	0.1361
276.87	20000.00	0.1392
277.62	15000.00	0.1374
277.69	100.00	0.1331
277.71	20000.00	0.1394
278.39	100.00	0.1330
278.48	5000.00	0.1344
278.65	10000.00	0.1366
296.02	20000.00	0.1358
296.14	5000.00	0.1312
296.19	15000.00	0.1344
296.20	100.00	0.1294
296.29	10000.00	0.1332
296.56	15000.00	0.1338
296.63	5000.00	0.1308
296.75	20000.00	0.1359
297.36	15000.00	0.1338
297.51	10000.00	0.1325
297.69	100.00	0.1293
298.13	20000.00	0.1356
298.26	5000.00	0.1309
298.36	15000.00	0.1340
298.41	100.00	0.1290
298.43	10000.00	0.1326
315.33	15000.00	0.1304
315.46	10000.00	0.1284
315.64	20000.00	0.1324
315.70	5000.00	0.1270
315.74	10000.00	0.1281
315.99	5000.00	0.1268
316.23	20000.00	0.1328
316.29	100.00	0.1248
316.91	15000.00	0.1310
317.25	10000.00	0.1284
317.28	100.00	0.1247
317.51	20000.00	0.1322
317.68	5000.00	0.1265
317.76	15000.00	0.1304

318.02	100.00	0.1250
318.11	20000.00	0.1318
336.49	100.00	0.1200
336.93	20000.00	0.1276
337.02	10000.00	0.1237
337.04	100.00	0.1201
337.39	5000.00	0.1223
337.46	10000.00	0.1236
337.82	5000.00	0.1222
337.85	5000.00	0.1219
337.87	15000.00	0.1257
338.66	100.00	0.1198
338.69	15000.00	0.1258
338.84	10000.00	0.1243
338.98	5000.00	0.1216
338.99	10000.00	0.1237
339.05	20000.00	0.1278
339.10	15000.00	0.1260
339.42	20000.00	0.1276
355.36	15000.00	0.1220
355.71	5000.00	0.1179
356.17	15000.00	0.1222
356.18	10000.00	0.1196
356.63	20000.00	0.1243
356.65	5000.00	0.1177
356.69	100.00	0.1148
356.99	100.00	0.1154
357.21	5000.00	0.1178
357.29	100.00	0.1155
357.31	15000.00	0.1219
357.40	20000.00	0.1245
357.48	10000.00	0.1194
357.52	10000.00	0.1197
358.21	20000.00	0.1244
375.68	20000.00	0.1197
375.73	10000.00	0.1158
375.83	100.00	0.1109
375.86	5000.00	0.1142
375.91	5000.00	0.1141
376.09	15000.00	0.1179
376.60	5000.00	0.1140
376.61	100.00	0.1111
376.71	10000.00	0.1162
376.83	10000.00	0.1155

377.29	15000.00	0.1185
377.41	15000.00	0.1178
377.45	20000.00	0.1197
377.52	100.00	0.1110
377.74	15000.00	0.1175
378.14	20000.00	0.1199

Reference

<https://www.doi.org/10.1021/je300778e>

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Liquid Density of 2 Methoxyethyl Acetate, 2 Ethylhexyl Acetate and Diethyl Sebacate at Temperatures from 298.15 to 363.15 K and Pressures up to 166 MPa	https://www.doi.org/10.1021/acs.jced.5b00385
Phase behavior of binary mixture for the isoalkyl acetate in supercritical carbon dioxide	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	https://www.doi.org/10.1016/j.fluid.2013.12.026
KDB Vapor Pressure Data:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1124
NIST Webbook:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1124
Joback Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103093&Units=SI
Crippen Method:	https://en.wikipedia.org/wiki/Joback_method
Liquid-liquid equilibria of water + acetic acid + 2-ethyl hexyl acetate ternary system	https://www.chemeo.com/doc/models/crippen_log10ws
Thermal Conductivity of Liquid 2-Methoxyethyl Acetate, 2-Ethylhexyl Acetate, and Diethyl Sebacate	https://www.doi.org/10.1016/j.fluid.2014.07.032
fuels: experiment and correlation:	https://www.doi.org/10.1021/je300778e
	https://www.doi.org/10.1016/j.fluid.2017.08.016

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
nfpaf:	NFPA Fire Rating

nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rho:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
vc:	Critical Volume

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