Acetic acid, octyl ester

Other names:	1-Octanol acetate
	1-Octyl acetate
	1-acetoxyoctane
	Acetate C-8
	Acetic acid n-octyl ester
	CAPRYLYL ACETATE
	NSC 67348
	OCTYL ACETATE
	OCTYL ALCOHOL ACETATE
	Octanol acetate
	ethanoic acid, octyl ester
	n-Octanyl acetate
	n-Octyl acetate
	n-Octyl ethanoate
	octyl ethanoate
Inchi:	InChI=1S/C10H20O2/c1-3-4-5-6-7-8-9-12-10(2)11/h3-9H2,1-2H3
InchiKey:	YLYBTZIQSIBWLI-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CCCCCCCCOC(C)=O
Mol. weight [g/mol]:	172.26
CAS:	112-14-1

Physical Properties

Property code	Value	Unit	Source
gf	-200.60	kJ/mol	Joback Method
hf	-494.53	kJ/mol	Joback Method
hfus	24.44	kJ/mol	Joback Method
hvap	60.70 ± 0.40	kJ/mol	NIST Webbook
hvap	61.70	kJ/mol	NIST Webbook
log10ws	-2.87		Crippen Method
logp	2.910		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
rinpol	1196.00		NIST Webbook
rinpol	1197.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1210.00		NIST Webbook

rinpol	1193.00	NIST Webbook
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ripol	1474.00		NIST Webbook
ripol	1468.00		NIST Webbook
ripol	1461.00		NIST Webbook
tb	484.65 ± 1.00	K	NIST Webbook
tb	486.15 ± 2.00	K	NIST Webbook
tb	483.20 ± 1.50	K	NIST Webbook
tb	480.15 ± 1.00	K	NIST Webbook
tb	483.20	K	NIST Webbook
tb	482.00 ± 4.00	K	NIST Webbook
tc	676.79	K	Joback Method
tf	234.65 ± 0.50	K	NIST Webbook
tf	291.65	K	KDB
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.00	J/mol×K	590.64	Joback Method
cpg	382.26	J/mol×K	533.21	Joback Method
cpg	368.11	J/mol×K	504.49	Joback Method
cpg	421.59	J/mol×K	619.36	Joback Method
cpg	433.67	J/mol×K	648.08	Joback Method
cpg	445.25	J/mol×K	676.79	Joback Method
cpg	395.89	J/mol×K	561.92	Joback Method
dvisc	0.0009057	Pa×s	351.24	Joback Method
dvisc	0.0032806	Pa×s	274.62	Joback Method

dvisc	0.0005753	Pa×s	389.56	Joback Method
dvisc	0.0003964	Pa×s	427.87	Joback Method
dvisc	0.0002904	Pa×s	466.18	Joback Method
dvisc	0.0002230	Pa×s	504.49	Joback Method
dvisc	0.0015931	Pa×s	312.93	Joback Method
hvapt	54.90	kJ/mol	375.50	NIST Webbook
hvapt	47.80	kJ/mol	408.50	NIST Webbook
pvap	0.04	kPa	309.20	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	0.03	kPa	306.10	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	0.03	kPa	303.10	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	0.02	kPa	300.10	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	0.02	kPa	297.00	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	0.01	kPa	294.00	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	9.48e-03	kPa	290.90	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates

pvap	7.28e-03	kPa	287.90	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	5.29e-03	kPa	284.80	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	4.13e-03	kPa	281.80	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	3.12e-03	kPa	278.70	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	1.97e-03	kPa	274.50	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	385.70	K	4.00	NIST Webbook

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol1125.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C112141&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates.	https://www.doi.org/10.1016/j.jct.2005.08.003
Parametric Analysis of Mandelic Acid Separation from Aqueous Solutions by Using Secondary Amine Mixture (Amberlite LA-2) in Various Diluents:	https://www.doi.org/10.1021/acs.jced.9b00169
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume