

Acetic acid, nonyl ester

Other names:	1-acetoxynonane
	Acetic acid n-nonyl ester
	Nonanol acetate
	Nonyl acetate
	Pelargonyl acetate
	ethanoic acid, nonyl ester
	n-Nonanyl acetate
	n-Nonyl acetate
	n-Nonyl ethanoate
	nonyl ethanoate
Inchi:	InChI=1S/C11H22O2/c1-3-4-5-6-7-8-9-10-13-11(2)12/h3-10H2,1-2H3
InchiKey:	GJQIMXVRFNLMTB-UHFFFAOYSA-N
Formula:	C11H22O2
SMILES:	CCCCCCCCCOC(C)=O
Mol. weight [g/mol]:	186.29
CAS:	143-13-5

Physical Properties

Property code	Value	Unit	Source
gf	-192.18	kJ/mol	Joback Method
hf	-515.17	kJ/mol	Joback Method
hfus	27.03	kJ/mol	Joback Method
hvap	66.80	kJ/mol	NIST Webbook
hvap	66.20 ± 0.20	kJ/mol	NIST Webbook
hvap	67.00	kJ/mol	NIST Webbook
log10ws	-3.29		Crippen Method
logp	3.300		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
rinpol	1308.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1314.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1311.00		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1300.00		NIST Webbook

rinpol	1295.00	NIST Webbook
rinpol	1293.00	NIST Webbook
rinpol	1293.00	NIST Webbook
rinpol	1291.00	NIST Webbook
rinpol	1292.00	NIST Webbook
rinpol	1290.00	NIST Webbook
rinpol	1308.00	NIST Webbook
rinpol	1308.00	NIST Webbook
rinpol	1291.00	NIST Webbook
rinpol	1311.00	NIST Webbook
rinpol	1311.00	NIST Webbook
rinpol	1292.00	NIST Webbook
rinpol	1284.00	NIST Webbook
rinpol	1292.00	NIST Webbook
rinpol	1296.00	NIST Webbook
rinpol	1292.00	NIST Webbook
rinpol	1290.00	NIST Webbook
rinpol	1293.00	NIST Webbook
rinpol	1295.00	NIST Webbook
rinpol	1292.00	NIST Webbook
rinpol	1309.00	NIST Webbook
rinpol	1289.39	NIST Webbook
rinpol	1310.45	NIST Webbook
rinpol	1291.70	NIST Webbook
rinpol	1292.00	NIST Webbook
rinpol	1292.00	NIST Webbook
rinpol	1293.00	NIST Webbook
rinpol	1293.00	NIST Webbook
rinpol	1285.00	NIST Webbook
rinpol	1289.80	NIST Webbook
rinpol	1290.00	NIST Webbook
rinpol	1295.00	NIST Webbook
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rinpol	1293.00	NIST Webbook
rinpol	1295.00	NIST Webbook
rinpol	1309.00	NIST Webbook
rinpol	1302.00	NIST Webbook
rinpol	1308.00	NIST Webbook
rinpol	1313.00	NIST Webbook
rinpol	1302.00	NIST Webbook
rinpol	1308.00	NIST Webbook
rinpol	1302.00	NIST Webbook
rinpol	1325.00	NIST Webbook
rinpol	1315.00	NIST Webbook

ripol	1304.00		NIST Webbook
ripol	1289.39		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1588.00		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1578.00		NIST Webbook
ripol	1573.00		NIST Webbook
ripol	1581.00		NIST Webbook
ripol	1584.00		NIST Webbook
ripol	1584.00		NIST Webbook
ripol	1560.00		NIST Webbook
ripol	1610.00		NIST Webbook
ripol	1588.00		NIST Webbook
ripol	1560.00		NIST Webbook
ripol	1581.00		NIST Webbook
ripol	1579.00		NIST Webbook
ripol	1602.20		NIST Webbook
ripol	1602.20		NIST Webbook
ripol	1587.00		NIST Webbook
ripol	1569.00		NIST Webbook
ripol	1574.00		NIST Webbook
ripol	1573.00		NIST Webbook
ripol	1581.00		NIST Webbook
ripol	1575.00		NIST Webbook
ripol	1585.00		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1581.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1560.00		NIST Webbook
ripol	1578.00		NIST Webbook
ripol	1587.00		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1617.00		NIST Webbook
ripol	1593.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1579.00		NIST Webbook
tb	497.00 ± 4.00	K	NIST Webbook
tc	698.36	K	Joback Method
tf	285.89	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.57	J/mol×K	698.36	Joback Method
cpg	430.19	J/mol×K	555.87	Joback Method
cpg	444.58	J/mol×K	584.37	Joback Method
cpg	458.41	J/mol×K	612.87	Joback Method
cpg	471.67	J/mol×K	641.36	Joback Method
cpg	484.39	J/mol×K	669.86	Joback Method
cpg	415.24	J/mol×K	527.37	Joback Method
dvisc	0.0032030	Pa×s	285.89	Joback Method
dvisc	0.0015281	Pa×s	326.14	Joback Method
dvisc	0.0008577	Pa×s	366.38	Joback Method
dvisc	0.0005398	Pa×s	406.63	Joback Method
dvisc	0.0003692	Pa×s	446.88	Joback Method
dvisc	0.0002689	Pa×s	487.12	Joback Method
dvisc	0.0002056	Pa×s	527.37	Joback Method
pvap	7.00e-04	kPa	276.70	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	8.60e-04	kPa	278.70	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	1.17e-03	kPa	281.80	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	1.59e-03	kPa	284.80	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	2.14e-03	kPa	287.80	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates

pvap	2.89e-03	kPa	290.90	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	3.89e-03	kPa	294.00	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	5.04e-03	kPa	297.00	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	6.72e-03	kPa	300.00	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	8.95e-03	kPa	303.10	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	0.01	kPa	306.10	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	0.01	kPa	309.20	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$

Coeff. A	1.45695e+01
Coeff. B	-4.15885e+03
Coeff. C	-7.60220e+01
Temperature range (K), min.	367.22
Temperature range (K), max.	525.24

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapour pressures and enthalpies of vaporization of a series of the linear alcohols:	https://www.doi.org/10.1016/j.jct.2005.08.003
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=C143135&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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