1-Octen-3-yl-acetate

Other names:	1-Octen-3-ol, acetate
	Amyl vinyl carbinol acetate
	Amyl vinyl carbinyl acetate
	1-Pentylallyl acetate
	1-Octenyl-3-acetate
	Oct-1-en-3-yl acetate
	Octen-3-yl acetate
	1-Oct-3-enylacetate
Inchi:	InChI=1S/C10H18O2/c1-4-6-7-8-10(5-2)12-9(3)11/h5,10H,2,4,6-8H2,1,3H3
InchiKey:	DOJDQRFOTHOBEK-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	C=CC(CCCCC)OC(C)=O
Mol. weight [g/mol]:	170.25
CAS:	2442-10-6

Physical Properties

Property code	Value	Unit	Source
gf	-115.20	kJ/mol	Joback Method
hf	-374.38	kJ/mol	Joback Method
hfus	19.64	kJ/mol	Joback Method
hvap	45.95	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.684		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2306.95	kPa	Joback Method
rinpol	1110.00		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1104.90		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1097.00		NIST Webbook

rinpol	1113.00	NIST Webbook
rinpol	1115.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1106.00	NIST Webbook
rinpol	1106.00	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1113.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1099.00	NIST Webbook
rinpol	1108.00	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1093.00	NIST Webbook
rinpol	1113.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1100.00	NIST Webbook
rinpol	1115.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1086.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1086.00	NIST Webbook
rinpol	1113.00	NIST Webbook
rinpol	1086.00	NIST Webbook
rinpol	1113.00	NIST Webbook
rinpol	1115.00	NIST Webbook
rinpol	1113.00	NIST Webbook
rinpol	1086.00	NIST Webbook
rinpol	1086.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1105.00	NIST Webbook
rinpol	1086.00	NIST Webbook
rinpol	1100.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1115.00	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1083.00	NIST Webbook
rinpol	1089.50	NIST Webbook
rinpol	1089.00	NIST Webbook
rinpol	1086.00	NIST Webbook
rinpol	1112.00	NIST Webbook
rinpol	1086.00	NIST Webbook
ripol	1365.00	NIST Webbook

ripol	1368.00		NIST Webbook
ripol	1380.00		NIST Webbook
ripol	1401.90		NIST Webbook
ripol	1401.90		NIST Webbook
ripol	1379.00		NIST Webbook
ripol	1392.00		NIST Webbook
ripol	1379.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1373.00		NIST Webbook
ripol	1379.00		NIST Webbook
ripol	1380.00		NIST Webbook
tb	500.73	K	Joback Method
tc	679.83	K	Joback Method
tf	257.86	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.06	J/mol×K	500.73	Joback Method
cpg	364.01	J/mol×K	530.58	Joback Method
cpg	377.40	J/mol×K	560.43	Joback Method
cpg	390.22	J/mol×K	590.28	Joback Method
cpg	402.50	J/mol×K	620.13	Joback Method
cpg	414.23	J/mol×K	649.98	Joback Method
cpg	425.43	J/mol×K	679.83	Joback Method
dvisc	0.0042919	Pa×s	257.86	Joback Method
dvisc	0.0018562	Pa×s	298.34	Joback Method
dvisc	0.0009808	Pa×s	338.82	Joback Method
dvisc	0.0005939	Pa×s	379.29	Joback Method
dvisc	0.0003961	Pa×s	419.77	Joback Method
dvisc	0.0002837	Pa×s	460.25	Joback Method
dvisc	0.0002145	Pa×s	500.73	Joback Method

Sources

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=C2442106&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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