

# 3-Octanol, acetate

Other names:	1-Ethylhexyl acetate
	3-Acetoxy octane
	3-Octanol, 3-acetate
	3-Octanyl acetate
	3-Octyl acetate
	Acetic acid, 1-ethylhexyl ester
	Amyl ethyl carbinyol acetate
	Octan-3-ol acetate
	octan-3-yl acetate
Inchi:	InChI=1S/C10H20O2/c1-4-6-7-8-10(5-2)12-9(3)11/h10H,4-8H2,1-3H3
InchiKey:	STZUZYMKSMSTOU-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CCCCC(CC)OC(C)=O
Mol. weight [g/mol]:	172.26
CAS:	4864-61-3

## 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	-2.98		Crippen Method
logp	2.908		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
rinpol	1123.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1122.00		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1113.00		NIST Webbook

rinpol	1126.50		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1123.00		NIST Webbook
ripol	1345.00		NIST Webbook
ripol	1340.00		NIST Webbook
ripol	1344.00		NIST Webbook
ripol	1345.00		NIST Webbook
ripol	1345.00		NIST Webbook
ripol	1333.00		NIST Webbook
ripol	1345.00		NIST Webbook
ripol	1345.00		NIST Webbook
ripol	1345.00		NIST Webbook
ripol	1345.00		NIST Webbook
ripol	1345.00		NIST Webbook
tb	504.05	K	Joback Method
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/molxK	504.05	Joback Method
cpg	435.35	J/molxK	650.52	Joback Method
cpg	423.03	J/molxK	621.22	Joback Method
cpg	410.17	J/molxK	591.93	Joback Method
cpg	396.77	J/molxK	562.64	Joback Method
cpg	382.82	J/molxK	533.34	Joback Method
cpg	447.14	J/molxK	679.81	Joback Method
dvisc	0.0002109	Paxs	504.05	Joback Method
dvisc	0.0002816	Paxs	463.31	Joback Method
dvisc	0.0003976	Paxs	422.57	Joback Method
dvisc	0.0006043	Paxs	381.84	Joback Method
dvisc	0.0010151	Paxs	341.10	Joback Method

dvisc	0.0019627	Paxs	300.36	Joback Method
dvisc	0.0046674	Paxs	259.62	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.40867e+01
Coeff. B	-3.85061e+03
Coeff. C	-6.90720e+01
Temperature range (K), min.	348.12
Temperature range (K), max.	507.88

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
Joback Method:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4864613&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4864613&amp;Units=SI</a>
The Yaws Handbook of Vapor Pressure:	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>

## 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

<b>pvap:</b>	Vapor pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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