

# Acetic acid n-octadecyl ester

<b>Other names:</b>	1-Octadecanol acetate 1-Octadecyl acetate Acetic acid, octadecyl ester Octadecanol acetate Octadecyl acetate Stearyl acetate n-Octadecyl acetate n-Octadecyl ethanoate
<b>Inchi:</b>	InChI=1S/C20H40O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-20(2)21/h3-19
<b>InchiKey:</b>	OIZXRZCQJDXPFO-UHFFFAOYSA-N
<b>Formula:</b>	C20H40O2
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCOC(C)=O
<b>Mol. weight [g/mol]:</b>	312.53
<b>CAS:</b>	822-23-1

## Physical Properties

Property code	Value	Unit	Source
gf	-116.40	kJ/mol	Joback Method
hf	-700.93	kJ/mol	Joback Method
hfus	50.34	kJ/mol	Joback Method
hvap	113.50	kJ/mol	NIST Webbook
log10ws	-7.06		Crippen Method
logp	6.811		Crippen Method
mcvol	300.100	ml/mol	McGowan Method
pc	1045.97	kPa	Joback Method
rinpol	2208.00		NIST Webbook
rinpol	2208.00		NIST Webbook
rinpol	2178.00		NIST Webbook
rinpol	2211.00		NIST Webbook
rinpol	2193.00		NIST Webbook
rinpol	2207.30		NIST Webbook
rinpol	2211.00		NIST Webbook
rinpol	2211.00		NIST Webbook
rinpol	2192.00		NIST Webbook
rinpol	2161.00		NIST Webbook
rinpol	2209.00		NIST Webbook
rinpol	2197.00		NIST Webbook

rinpol	2197.00		NIST Webbook
rinpol	2205.00		NIST Webbook
rinpol	2208.00		NIST Webbook
rinpol	2161.00		NIST Webbook
rinpol	2211.00		NIST Webbook
rinpol	2209.00		NIST Webbook
ripol	2516.00		NIST Webbook
ripol	2521.00		NIST Webbook
ripol	2521.00		NIST Webbook
ripol	2516.00		NIST Webbook
tb	733.29	K	Joback Method
tc	904.52	K	Joback Method
tf	305.80 ± 0.60	K	NIST Webbook
vc	1.179	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.52	J/mol×K	733.29	Joback Method
cpg	928.17	J/mol×K	761.83	Joback Method
cpg	946.91	J/mol×K	790.37	Joback Method
cpg	964.76	J/mol×K	818.91	Joback Method
cpg	981.74	J/mol×K	847.45	Joback Method
cpg	997.86	J/mol×K	875.99	Joback Method
cpg	1013.17	J/mol×K	904.52	Joback Method
dvisc	0.0016619	Paxs	387.32	Joback Method
dvisc	0.0007053	Paxs	444.98	Joback Method
dvisc	0.0003644	Paxs	502.64	Joback Method
dvisc	0.0002156	Paxs	560.30	Joback Method
dvisc	0.0001407	Paxs	617.97	Joback Method
dvisc	0.0000988	Paxs	675.63	Joback Method
dvisc	0.0000733	Paxs	733.29	Joback Method
hvapt	94.30	kJ/mol	420.50	NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	452.50 ± 0.50	K	0.30	NIST Webbook

# Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.57805e+01
Coeff. B	-1.03474e+04
Coeff. C	-1.36626e+02
Temperature range (K), min.	542.52
Temperature range (K), max.	642.14

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C822231&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C822231&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<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>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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