Acetic acid, octadecyl ester

Other names:	1-Octadecanol acetate
	1-Octadecyl acetate
	Octadecanol acetate
	Octadecyl acetate
	Stearyl acetate
	n-Octadecyl acetate
	n-Octadecyl ethanoate
Inchi:	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
InchiKey:	OIZXRZCQJDXPFO-UHFFFAOYSA-N
Formula:	C20H40O2
SMILES:	CCCCCCCCCCCCCCCCCCOC(C)=O
Mol. weight [g/mol]:	312.54
CAS:	822-23-1

Physical Properties

Property code	Value	Unit	Source
af	0.9656		Cheméo Relay (1.0)
gf	-116.40	kJ/mol	Joback Method
hf	-783.84	kJ/mol	Cheméo Relay (1.0)
hfus	50.34	kJ/mol	Joback Method
hvap	113.50	kJ/mol	NIST Webbook
ie	9.78	eV	Cheméo Relay (1.0)
log10ws	-7.06		Cheméo Relay (1.0)
logp	6.811		Crippen Method
mcvol	300.100	ml/mol	McGowan Method
pc	1045.97	kPa	Joback Method
rinpol	2192.00		NIST Webbook
rinpol	2205.00		NIST Webbook
rinpol	2178.00		NIST Webbook
rinpol	2211.00		NIST Webbook
rinpol	2208.00		NIST Webbook
rinpol	2207.30		NIST Webbook
rinpol	2211.00		NIST Webbook
rinpol	2211.00		NIST Webbook
rinpol	2193.00		NIST Webbook
rinpol	2209.00		NIST Webbook
rinpol	2209.00		NIST Webbook

rinpol	2197.00		NIST Webbook
rinpol	2197.00		NIST Webbook
rinpol	2208.00		NIST Webbook
rinpol	2208.00		NIST Webbook
rinpol	2161.00		NIST Webbook
rinpol	2211.00		NIST Webbook
rinpol	2161.00		NIST Webbook
ripol	2521.00		NIST Webbook
ripol	2521.00		NIST Webbook
ripol	2516.00		NIST Webbook
ripol	2516.00		NIST Webbook
tb	594.24	K	Cheméo Relay (1.0)
tc	771.63	K	Cheméo Relay (1.0)
tf	305.80 ± 0.60	K	NIST Webbook
vc	1.187	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.52	J/mol×K	733.29	Joback Method
cpg	1013.17	J/mol×K	904.52	Joback Method
cpg	997.86	J/mol×K	875.99	Joback Method
cpg	981.74	J/mol×K	847.45	Joback Method
cpg	964.76	J/mol×K	818.91	Joback Method
cpg	946.91	J/mol×K	790.37	Joback Method
cpg	928.17	J/mol×K	761.83	Joback Method
dvisc	0.0002156	Pa×s	560.31	Joback Method
dvisc	0.0000733	Pa×s	733.29	Joback Method
dvisc	0.0000988	Pa×s	675.63	Joback Method
dvisc	0.0001407	Pa×s	617.97	Joback Method
dvisc	0.0016619	Pa×s	387.32	Joback Method
dvisc	0.0003644	Pa×s	502.64	Joback Method
dvisc	0.0007053	Pa×s	444.98	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(Pvp) = 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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C822231&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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

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

Legend

af: Acentric Factor
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
ie: Ionization energy

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