Lauryl acetate

Other names:	1-Dodecanol acetate
	Acetic acid, dodecyl ester
	Dodecan-1-ol, acetate
	Dodecan-1-yl acetate
	Dodecanol acetate
	Dodecanyl acetate
	Dodecyl acetate
	Dodecyl alcohol, acetate
	NSC 67366
	dodecyl ethanoate
	n-Dodecyl acetate
	n-Dodecyl ethanoate
Inchi:	InChI=1S/C14H28O2/c1-3-4-5-6-7-8-9-10-11-12-13-16-14(2)15/h3-13H2,1-2H3
InchiKey:	VZWGRQBCURJOMT-UHFFFAOYSA-N
Formula:	C14H28O2
SMILES:	CCCCCCCCCCCCOC(C)=O
Mol. weight [g/mol]:	228.37
CAS:	112-66-3

Physical Properties

Property code	Value	Unit	Source
gf	-166.92	kJ/mol	Joback Method
hf	-577.09	kJ/mol	Joback Method
hfus	34.80	kJ/mol	Joback Method
hvap	81.80	kJ/mol	NIST Webbook
hvap	79.60 ± 0.30	kJ/mol	NIST Webbook
log10ws	-4.55		Crippen Method
logp	4.470		Crippen Method
mcvol	215.560	ml/mol	McGowan Method
pc	1579.71	kPa	Joback Method
rinpol	1610.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1613.00		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1592.00		NIST Webbook

rinpol	1605.90	NIST Webbook
rinpol	1597.00	NIST Webbook
rinpol	1585.00	NIST Webbook
rinpol	1606.00	NIST Webbook
rinpol	1588.00	NIST Webbook
rinpol	1606.00	NIST Webbook
rinpol	1592.00	NIST Webbook
rinpol	1576.00	NIST Webbook
rinpol	1606.00	NIST Webbook
rinpol	1596.00	NIST Webbook
rinpol	1594.00	NIST Webbook
rinpol	1594.00	NIST Webbook
rinpol	1591.00	NIST Webbook
rinpol	1576.00	NIST Webbook
rinpol	1589.60	NIST Webbook
rinpol	1562.00	NIST Webbook
rinpol	1587.00	NIST Webbook
rinpol	1620.00	NIST Webbook
rinpol	1611.00	NIST Webbook
rinpol	1609.00	NIST Webbook
rinpol	1610.00	NIST Webbook
rinpol	1595.00	NIST Webbook
rinpol	1608.50	NIST Webbook
rinpol	1605.90	NIST Webbook
rinpol	1580.00	NIST Webbook
ripol	1900.00	NIST Webbook
ripol	1882.00	NIST Webbook
ripol	1891.00	NIST Webbook
ripol	1893.00	NIST Webbook
ripol	1893.00	NIST Webbook
ripol	1880.00	NIST Webbook
ripol	1876.00	NIST Webbook
ripol	1893.00	NIST Webbook
ripol	1893.00	NIST Webbook
ripol	1883.00	NIST Webbook
ripol	1884.00	NIST Webbook
ripol	1882.00	NIST Webbook
ripol	1895.00	NIST Webbook
ripol	1880.00	NIST Webbook
ripol	1868.00	NIST Webbook
ripol	1896.00	NIST Webbook
ripol	1898.00	NIST Webbook
ripol	1880.00	NIST Webbook
ripol	1880.00	NIST Webbook

tb	538.20	K	NIST Webbook
tc	764.02	K	Joback Method
tf	319.70	K	Joback Method
vc	0.844	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.02	J/mol×K	596.01	Joback Method
cpg	600.10	J/mol×K	652.01	Joback Method
cpg	615.63	J/mol×K	680.02	Joback Method
cpg	630.49	J/mol×K	708.02	Joback Method
cpg	644.71	J/mol×K	736.02	Joback Method
cpg	658.29	J/mol×K	764.02	Joback Method
cpg	583.90	J/mol×K	624.01	Joback Method
dvisc	0.0012632	Pa×s	365.75	Joback Method
dvisc	0.0006860	Pa×s	411.80	Joback Method
dvisc	0.0004212	Pa×s	457.86	Joback Method
dvisc	0.0002827	Pa×s	503.91	Joback Method
dvisc	0.0002029	Pa×s	549.96	Joback Method
dvisc	0.0001532	Pa×s	596.01	Joback Method
dvisc	0.0027735	Pa×s	319.70	Joback Method
hvapt	70.50	kJ/mol	469.00	NIST Webbook
pvap	5.97e-03	kPa	333.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	4.56e-03	kPa	330.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	3.56e-03	kPa	327.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates

pvap	2.80e-03	kPa	324.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	2.08e-03	kPa	321.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	1.63e-03	kPa	318.20	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	1.19e-03	kPa	315.20	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	9.00e-04	kPa	312.10	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	6.70e-04	kPa	309.20	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	4.90e-04	kPa	306.10	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	3.70e-04	kPa	303.10	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	2.40e-04	kPa	299.00	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates

pvap	1.70e-04	kPa	296.00	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	1.10e-04	kPa	291.90	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	8.00e-05	kPa	288.90	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	423.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.81806e+01
Coeff. B	-6.01367e+03
Coeff. C	-9.99300e+01
Temperature range (K), min.	436.02
Temperature range (K), max.	567.22

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C112663&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-acetates.	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

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
hvapt:	Enthalpy of vaporization at a given temperature
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