1-Undecanol, acetate

Other names:	Acetic acid undecyl ester
	Undecyl acetate
	Undecyl alcohol, acetate
	acetic acid, undecyl ester
	n-Undecyl acetate
	undecanyl acetate
	undecyl ethanoate
Inchi:	InChI=1S/C13H26O2/c1-3-4-5-6-7-8-9-10-11-12-15-13(2)14/h3-12H2,1-2H3
InchiKey:	CKQGCFFDQIFZFA-UHFFFAOYSA-N
Formula:	C13H26O2
SMILES:	CCCCCCCCCCCOC(C)=O
Mol. weight [g/mol]:	214.34
CAS:	1731-81-3

Physical Properties

Property code	Value	Unit	Source
gf	-175.34	kJ/mol	Joback Method
hf	-556.45	kJ/mol	Joback Method
hfus	32.21	kJ/mol	Joback Method
hvap	53.69	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	4.080		Crippen Method
mcvol	201.470	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
rinpol	1493.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1507.60		NIST Webbook
rinpol	1487.00		NIST Webbook
ripol	1802.00		NIST Webbook
ripol	1775.00		NIST Webbook
tb	573.13	K	Joback Method
tc	741.92	K	Joback Method
tf	308.43	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.80	J/mol×K	573.13	Joback Method
cpg	546.77	J/mol×K	629.39	Joback Method
cpg	561.79	J/mol×K	657.52	Joback Method
cpg	576.19	J/mol×K	685.66	Joback Method
cpg	589.97	J/mol×K	713.79	Joback Method
cpg	603.14	J/mol×K	741.92	Joback Method
cpg	531.11	J/mol×K	601.26	Joback Method
dvisc	0.0013589	Pa×s	352.55	Joback Method
dvisc	0.0007456	Pa×s	396.66	Joback Method
dvisc	0.0004613	Pa×s	440.78	Joback Method
dvisc	0.0003115	Pa×s	484.90	Joback Method
dvisc	0.0002245	Pa×s	529.01	Joback Method
dvisc	0.0029408	Pa×s	308.43	Joback Method
dvisc	0.0001702	Pa×s	573.13	Joback Method
pvap	0.01	kPa	329.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	8.29e-03	kPa	326.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	6.32e-03	kPa	323.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	4.99e-03	kPa	320.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates

pvap	3.76e-03	kPa	317.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	2.98e-03	kPa	314.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	2.26e-03	kPa	311.20	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	1.67e-03	kPa	308.20	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	1.23e-03	kPa	305.20	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	9.50e-04	kPa	302.10	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	7.10e-04	kPa	299.00	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	4.90e-04	kPa	296.00	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	3.70e-04	kPa	292.90	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates

pvap	2.40e-04	kPa	288.90	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.76319e+01
Coeff. B	-5.64569e+03
Coeff. C	-9.38140e+01
Temperature range (K), min.	419.32
Temperature range (K), max.	552.05

Sources

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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1133.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1731813&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

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
pvap:	Vapor 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