Acetic acid, decyl ester

Other names:	1-Decanol acetate ACETIC ACID Acetate C 10 Acetic acid, n-decyl ester DECYL ACETATE DECYL ESTER Decanol acetate Decyl alcohol, acetate Decyl ester of acetic acid N-DECYL ETHANOATE decyl ethanoate n-Decyl acetate
Inchi:	InChI=1S/C12H24O2/c1-3-4-5-6-7-8-9-10-11-14-12(2)13/h3-11H2,1-2H3
InchiKey:	NUPSHWCALHZGOV-UHFFFAOYSA-N
Formula:	C12H24O2
SMILES:	CCCCCCCCCCOC(C)=O
Mol. weight [g/mol]:	200.32
CAS:	112-17-4

Physical Properties

Property code	Value	Unit	Source
gf	-183.76	kJ/mol	Joback Method
hf	-535.81	kJ/mol	Joback Method
hfus	29.62	kJ/mol	Joback Method
hvap	70.20 ± 0.30	kJ/mol	NIST Webbook
hvap	71.60	kJ/mol	NIST Webbook
log10ws	-3.71		Crippen Method
logp	3.690		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	1391.00		NIST Webbook
rinpol	1410.32		NIST Webbook
rinpol	1391.30		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1384.00		NIST Webbook

rinpol	1389.20	NIST Webbook
rinpol	1399.00	NIST Webbook
rinpol	1385.00	NIST Webbook
rinpol	1419.00	NIST Webbook
rinpol	1417.00	NIST Webbook
rinpol	1394.00	NIST Webbook
rinpol	1409.00	NIST Webbook
rinpol	1409.00	NIST Webbook
rinpol	1395.00	NIST Webbook
rinpol	1408.00	NIST Webbook
rinpol	1404.00	NIST Webbook
rinpol	1394.00	NIST Webbook
rinpol	1408.00	NIST Webbook
rinpol	1404.00	NIST Webbook
rinpol	1408.00	NIST Webbook
rinpol	1408.00	NIST Webbook
rinpol	1389.27	NIST Webbook
rinpol	1410.00	NIST Webbook
rinpol	1409.00	NIST Webbook
rinpol	1404.00	NIST Webbook
rinpol	1408.00	NIST Webbook
rinpol	1393.00	NIST Webbook
rinpol	1394.00	NIST Webbook
rinpol	1395.00	NIST Webbook
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ripol	1662.00		NIST Webbook
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ripol	1662.00		NIST Webbook
ripol	1674.00		NIST Webbook
ripol	1679.00		NIST Webbook
ripol	1678.00		NIST Webbook
ripol	1683.00		NIST Webbook
ripol	1669.00		NIST Webbook
tb	517.15 ± 1.00	K	NIST Webbook
tc	720.05	K	Joback Method
tf	297.16	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.17	J/mol×K	550.25	Joback Method
cpg	479.84	J/mol×K	578.55	Joback Method
cpg	494.90	J/mol×K	606.85	Joback Method
cpg	509.36	J/mol×K	635.15	Joback Method
cpg	523.23	J/mol×K	663.45	Joback Method
cpg	536.51	J/mol×K	691.75	Joback Method
cpg	549.22	J/mol×K	720.05	Joback Method
dvisc	0.0030867	Pa×s	297.16	Joback Method
dvisc	0.0014485	Pa×s	339.34	Joback Method
dvisc	0.0008035	Pa×s	381.52	Joback Method
dvisc	0.0005012	Pa×s	423.70	Joback Method

dvisc	0.0003406	Pa×s	465.89	Joback Method
dvisc	0.0002467	Pa×s	508.07	Joback Method
dvisc	0.0001878	Pa×s	550.25	Joback Method
hvapt	56.30	kJ/mol	487.50	NIST Webbook
hvapt	72.00	kJ/mol	306.00	NIST Webbook
hvapt	61.90	kJ/mol	439.00	NIST Webbook
pvap	0.01	kPa	318.50	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	8.37e-03	kPa	315.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	6.66e-03	kPa	312.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	5.04e-03	kPa	309.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	3.95e-03	kPa	306.40	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	2.92e-03	kPa	303.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	2.28e-03	kPa	300.30	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates

pvap	1.67e-03	kPa	297.00	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	1.21e-03	kPa	294.00	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	9.00e-04	kPa	290.90	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	6.60e-04	kPa	287.80	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	4.80e-04	kPa	284.80	Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates
pvap	0.01	kPa	321.50	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	1.69025e+01
Coeff. B	-5.20250e+03
Coeff. C	-8.76980e+01
Temperature range (K), min.	400.82
Temperature range (K), max.	536.54

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.91628e+01
Coeff. B	-7.43974e+03
Coeff. C	-2.54488e-04
Coeff. D	2.79788e-10
Temperature range (K), min.	363.15
Temperature range (K), max.	449.15

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1130
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1130.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112174&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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