Formic acid, pentyl ester

Other names:	1-pentyl formate
	3-PENTANOL FORMATE
	Amyl formate
	N-AMYL FORMATE
	PENTYL FORMATE
	UN 1109
	formic acid, amyl ester
	methanoic acid, pentyl ester
	n-Pentyl formate
	n-Pentyl methanoate
	pentyl methanoate
Inchi:	InChI=1S/C6H12O2/c1-2-3-4-5-8-6-7/h6H,2-5H2,1H3
InchiKey:	DIQMPQMYFZXDAX-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CCCCCOC=O
Mol. weight [g/mol]:	116.16
CAS:	638-49-3

Physical Properties

Property code	Value	Unit	Source
af	0.5380		KDB
gf	-204.88	kJ/mol	Joback Method
hf	-384.97	kJ/mol	Joback Method
hfus	14.77	kJ/mol	Joback Method
hvap	38.08	kJ/mol	Joback Method
log10ws	-1.20		Crippen Method
logp	1.350		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=1)		KDB
pc	3460.00	kPa	KDB
pc	3457.00 ± 303.98	kPa	NIST Webbook
rhoc	282.26 ± 4.65	kg/m3	NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	827.00		NIST Webbook

rinpol	810.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	795.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	797.00		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	797.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	781.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	826.00		NIST Webbook
rinpol	827.00		NIST Webbook
ripol	1187.00		NIST Webbook
ripol	1187.00		NIST Webbook
tb	405.00 ± 1.50	K	NIST Webbook
tb	380.00 ± 2.00	K	NIST Webbook
tb	405.50 ± 1.00	K	NIST Webbook
tb	403.60 ± 1.50	K	NIST Webbook
tb	395.70 ± 1.00	K	NIST Webbook
tb	405.12	K	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
tb	393.15 ± 1.00	K	NIST Webbook
tb	405.25 ± 1.00	K	NIST Webbook
tb	403.60	K	KDB
tc	576.00	K	KDB
tc	575.80 ± 4.00	K	NIST Webbook
tf	199.60	K	KDB
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.33	J/mol×K	551.66	Joback Method
cpg	201.68	J/mol×K	407.76	Joback Method
cpg	211.20	J/mol×K	436.54	Joback Method
cpg	220.43	J/mol×K	465.32	Joback Method
cpg	229.36	J/mol×K	494.10	Joback Method
cpg	238.00	J/mol×K	522.88	Joback Method
cpg	254.37	J/mol×K	580.45	Joback Method
dvisc	0.0017464	Pa×s	252.64	Joback Method
dvisc	0.0033772	Pa×s	221.61	Joback Method
dvisc	0.0002910	Pa×s	407.76	Joback Method
dvisc	0.0010432	Pa×s	283.66	Joback Method
dvisc	0.0006898	Pa×s	314.69	Joback Method
dvisc	0.0004913	Pa×s	345.71	Joback Method
dvisc	0.0003700	Pa×s	376.74	Joback Method
pvap	60.50	kPa	387.67	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	2.76	kPa	313.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	101.30	kPa	405.12	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	93.45	kPa	402.19	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	86.56	kPa	399.55	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane

pvap	80.16	kPa	396.89	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	73.50	kPa	394.01	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	68.46	kPa	391.65	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	2.37	kPa	310.70	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	55.79	kPa	385.08	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	49.42	kPa	381.35	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	44.06	kPa	377.87	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	39.15	kPa	374.41	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	33.67	kPa	370.04	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	60.00	kPa	387.46	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane

pvap	60.00	kPa	387.40	Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane
pvap	2.05	kPa	308.00	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	1.78	kPa	305.60	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	1.57	kPa	303.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	1.16	kPa	298.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.85	kPa	293.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.61	kPa	288.20	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.43	kPa	283.20	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.37	kPa	281.00	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.37	kPa	281.00	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.30	kPa	278.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.30	kPa	278.30	Vapour pressures and enthalpies of vaporization of aliphatic esters

pvap	0.25	kPa	275.70	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.23	kPa	274.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.23	kPa	274.20	Vapour pressures and enthalpies of vaporization of aliphatic esters
rhol	902.00	kg/m3	273.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.65215e+01
Coeff. B	-4.09248e+03
Coeff. C	-5.41850e+01
Temperature range (K), min.	306.28
Temperature range (K), max.	419.26

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.89999e+01
Coeff. B	-9.05957e+03
Coeff. C	-1.21588e+01
Coeff. D	6.07490e-06
Temperature range (K), min.	199.65
Temperature range (K), max.	576.00

Sources

Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) V. Hex and Vex for 25 binary mixtures {xCu-1H2u-1CO2CH3 + (1-x)a,x-ClCH2(CH2)v-2CH2Cl}, where u = 1 to 5, a = 1 and v = x = 2 to 6: https://www.doi.org/10.1016/j.jct.2006.10.008

Vapor Liquid Equilibria Measurements for the Five Linear C6 Esters with n-Octane:	https://www.doi.org/10.1021/acs.jced.5b01058
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Assessment, measurement and correlation of (vapour + liquid) equilibrium of (carbon dioxide + butyl, isobutyl, and amyl formate) systems:	https://www.doi.org/10.1016/j.jct.2013.05.017
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1083.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C638493&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1083
Vapour pressures and enthalpies of vaporization of aliphatic esters:	https://www.doi.org/10.1016/j.fluid.2012.08.003

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density
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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.