Propanoic acid, pentyl ester

Other names:	AMYL PROPIONATE
	Amyl propanoate
	N-PENTYL PROPANOATE
	NSC 7931
	Pentyl propanate
	Pentyl propanoate
	Pentyl propionate
	Propionic acid, pentyl ester
	ethyl butyrate
	n-Amyl n-propionate
	n-Amyl propionate
	n-Pentyl propionate
	propionic acid, amyl ester
Inchi:	InChI=1S/C8H16O2/c1-3-5-6-7-10-8(9)4-2/h3-7H2,1-2H3
InchiKey:	TWSRVQVEYJNFKQ-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCCCCOC(=O)CC
Mol. weight [g/mol]:	144.21
CAS:	624-54-4

Physical Properties

Property code	Value	Unit	Source
gf	-217.44	kJ/mol	Joback Method
hf	-453.25	kJ/mol	Joback Method
hfus	19.26	kJ/mol	Joback Method
hvap	42.56	kJ/mol	Joback Method
log10ws	-1.28		Aqueous Solubility Prediction Method
log10ws	-1.28		Estimated Solubility Method
logp	2.130		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
rinpol	987.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	990.00		NIST Webbook

rinpol	989.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	1001.50		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	998.00		NIST Webbook
rinpol	949.00		NIST Webbook
rinpol	950.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	972.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	972.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	980.41		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	990.50		NIST Webbook
ripol	1236.00		NIST Webbook
ripol	1247.00		NIST Webbook
ripol	1239.00		NIST Webbook
ripol	1208.00		NIST Webbook
ripol	1257.00		NIST Webbook
ripol	1255.00		NIST Webbook
ripol	1234.00		NIST Webbook
ripol	1235.00		NIST Webbook
ripol	1288.00		NIST Webbook
ripol	1210.00		NIST Webbook
ripol	1238.00		NIST Webbook
ripol	1258.00		NIST Webbook
tb	441.90	K	KDB
tb	441.80	K	NIST Webbook
tb	441.90 ± 1.00	K	NIST Webbook
tb	441.80 ± 1.00	K	NIST Webbook
tb	437.00 ± 2.00	K	NIST Webbook
tc	633.80	K	Joback Method
tf	200.05	K	Aqueous Solubility Prediction Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.64	J/mol×K	604.62	Joback Method
cpg	279.70	J/mol×K	458.73	Joback Method
cpg	291.94	J/mol×K	487.91	Joback Method
cpg	303.75	J/mol×K	517.09	Joback Method
cpg	315.14	J/mol×K	546.26	Joback Method
cpg	326.10	J/mol×K	575.44	Joback Method
cpg	346.77	J/mol×K	633.80	Joback Method
cpl	245.20	J/mol×K	298.15	NIST Webbook
dvisc	0.0002540	Pa×s	458.73	Joback Method
dvisc	0.0032831	Pa×s	252.08	Joback Method
dvisc	0.0016585	Pa×s	286.52	Joback Method
dvisc	0.0009701	Pa×s	320.96	Joback Method
dvisc	0.0006296	Pa×s	355.40	Joback Method
dvisc	0.0004410	Pa×s	389.85	Joback Method
dvisc	0.0003273	Pa×s	424.29	Joback Method
hvapt	44.10	kJ/mol	357.50	NIST Webbook
pvap	1.29	kPa	328.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.03	kPa	274.10	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.03	kPa	275.50	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.04	kPa	278.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.05	kPa	280.90	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.06	kPa	283.40	Vapour pressures and enthalpies of vaporization of aliphatic esters

pvap	0.09	kPa	288.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.14	kPa	293.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.20	kPa	298.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.28	kPa	303.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.39	kPa	308.20	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.53	kPa	313.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.72	kPa	318.50	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.84	kPa	320.70	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.96	kPa	323.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	1.10	kPa	325.60	Vapour pressures and enthalpies of vaporization of aliphatic esters
rhol	848.98	kg/m3	318.15	Thermodynamic properties of (an ester + and alkane). XVII. Experimental He and Ve values for (an alkyl propanoate + an alkane) at 318.15K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51106e+01
Coeff. B	-3.96398e+03
Coeff. C	-6.39980e+01
Temperature range (K), min.	331.42
Temperature range (K), max.	468.52

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.11415e+01
Coeff. B	-5.46526e+03
Coeff. C	-6.04912e-01
Coeff. D	-1.53384e-06
Temperature range (K), min.	294.15
Temperature range (K), max.	604.15

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1105

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Vapour pressures and enthalpies of vaporization of aliphatic esters: https://www.doi.org/10.1016/j.fluid.2012.08.003

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

Thermodynamic properties of (an ester + and alkane). XVII. Experimental He and Ve values for (an alkyl propanoate + an alkane) at 318.15K: https://www.doi.org/10.1016/j.jct.2004.12.014

KDB: https://www.cheric.org/files/research/kdb/mol/mol1105.mol

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C624544&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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
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