Pentanoic acid, propyl ester

Other names:	Propyl pentanoate
	Propyl valerate
	Valeric acid, propyl ester
	n-Propyl n-valerate
	n-propyl pentanoate
Inchi:	InChI=1S/C8H16O2/c1-3-5-6-8(9)10-7-4-2/h3-7H2,1-2H3
InchiKey:	ROJKPKOYARNFNB-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCCCC(=O)OCCC
Mol. weight [g/mol]:	144.21
CAS:	141-06-0

Physical Properties

Property code	Value	Unit	Source
chl	-4851.80 ± 1.30	kJ/mol	NIST Webbook
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	-2.03		Crippen Method
logp	2.130		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
rinpol	971.00		NIST Webbook
rinpol	971.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	979.00		NIST Webbook
rinpol	971.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	971.00		NIST Webbook
ripol	1217.00		NIST Webbook
ripol	1233.00		NIST Webbook
ripol	1200.00		NIST Webbook
tb	440.70 ± 1.00	K	NIST Webbook
tb	440.70	K	NIST Webbook
tb	440.70 ± 2.00	K	NIST Webbook

tc	633.80	K	Joback Method
tf	252.08	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.77	J/mol×K	633.80	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	336.64	J/mol×K	604.62	Joback Method
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	40.00	kJ/mol	293.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49746e+01
Coeff. B	-3.90482e+03
Coeff. C	-6.36510e+01
Temperature range (K), min.	329.52
Temperature range (K), max.	467.75

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1100.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C141060&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

Legend

chl:	Standard liquid enthalpy of combustion
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