Pentanoic acid, 1-methylethyl ester

Other names:	Isopropyl pentanoate
	Isopropyl valerate
	Pentanoic acid isopropyl ester
	Valeric acid, isopropyl ester
	n-C4H9C(O)OCH(CH3)2
Inchi:	InChI=1S/C8H16O2/c1-4-5-6-8(9)10-7(2)3/h7H,4-6H2,1-3H3
InchiKey:	OCAIYHCKLADPEG-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCCCC(=O)OC(C)C
Mol. weight [g/mol]:	144.21
CAS:	18362-97-5

Physical Properties

Property code	Value	Unit	Source
chl	-4842.60 ± 2.90	kJ/mol	NIST Webbook
gf	-219.88	kJ/mol	Joback Method
hf	-545.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-592.00 ± 3.00	kJ/mol	NIST Webbook
hfus	15.74	kJ/mol	Joback Method
hvap	47.00	kJ/mol	NIST Webbook
hvap	47.00 ± 1.00	kJ/mol	NIST Webbook
log10ws	-2.15		Crippen Method
logp	2.128		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	924.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	924.00		NIST Webbook
ripol	1135.00		NIST Webbook
ripol	1125.00		NIST Webbook
ripol	1135.00		NIST Webbook
tb	458.29	K	Joback Method

tc	637.16	K	Joback Method
tf	237.08	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.57	J/mol×K	637.16	Joback Method
cpg	279.83	J/mol×K	458.29	Joback Method
cpg	292.41	J/mol×K	488.10	Joback Method
cpg	304.54	J/mol×K	517.91	Joback Method
cpg	316.22	J/mol×K	547.72	Joback Method
cpg	327.44	J/mol×K	577.53	Joback Method
cpg	338.23	J/mol×K	607.34	Joback Method
dvisc	0.0002420	Pa×s	458.29	Joback Method
dvisc	0.0048246	Pa×s	237.08	Joback Method
dvisc	0.0020946	Pa×s	273.95	Joback Method
dvisc	0.0011084	Pa×s	310.82	Joback Method
dvisc	0.0006713	Pa×s	347.69	Joback Method
dvisc	0.0004476	Pa×s	384.55	Joback Method
dvisc	0.0003204	Pa×s	421.42	Joback Method
hvapt	38.00	kJ/mol	293.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46046e+01
Coeff. B	-3.74603e+03
Coeff. C	-6.08710e+01
Temperature range (K), min.	322.52
Temperature range (K), max.	463.97

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18362975&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
hfl:	Liquid phase 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