Pentanoic acid, 2-methylpropyl ester

Other names:	2-METHYLPROPYL VALERATE
	2-Methyl-1-propyl n-valerate
	ISOBUTYL PENTANOATE
	ISOBUTYL VALERINATE
	Isobutyl valerate
	Valeric acid, isobutyl ester
Inchi:	InChI=1S/C9H18O2/c1-4-5-6-9(10)11-7-8(2)3/h8H,4-7H2,1-3H3
InchiKey:	ADNADZOSMJDVIS-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCCCC(=O)OCC(C)C
Mol. weight [g/mol]:	158.24
CAS:	10588-10-0

Physical Properties

Property code	Value	Unit	Source
chl	-5486.50 ± 3.30	kJ/mol	NIST Webbook
gf	-211.46	kJ/mol	Joback Method
hf	-569.00 ± 4.00	kJ/mol	NIST Webbook
hfl	-620.00 ± 3.00	kJ/mol	NIST Webbook
hfus	18.33	kJ/mol	Joback Method
hvap	51.00	kJ/mol	NIST Webbook
hvap	51.00 ± 1.00	kJ/mol	NIST Webbook
log10ws	-2.21		Crippen Method
logp	2.376		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	1027.00		NIST Webbook
rinpol	1009.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	1009.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	1027.00		NIST Webbook
ripol	1252.00		NIST Webbook

ripol	1252.00		NIST Webbook
ripol	1253.00		NIST Webbook
tb	481.17	K	Joback Method
tc	658.49	K	Joback Method
tf	248.35	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.06	J/mol×K	481.17	Joback Method
cpg	336.66	J/mol×K	510.72	Joback Method
cpg	349.76	J/mol×K	540.28	Joback Method
cpg	362.35	J/mol×K	569.83	Joback Method
cpg	374.44	J/mol×K	599.38	Joback Method
cpg	386.04	J/mol×K	628.93	Joback Method
cpg	397.15	J/mol×K	658.49	Joback Method
dvisc	0.0047844	Pa×s	248.35	Joback Method
dvisc	0.0020429	Pa×s	287.15	Joback Method
dvisc	0.0010682	Pa×s	325.96	Joback Method
dvisc	0.0006412	Pa×s	364.76	Joback Method
dvisc	0.0004246	Pa×s	403.56	Joback Method
dvisc	0.0003022	Pa×s	442.37	Joback Method
dvisc	0.0002272	Pa×s	481.17	Joback Method
hvapt	41.00	kJ/mol	293.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.77538e+00
Coeff. B	-5.00764e+03
Coeff. C	1.03362e+00
Coeff. D	-5.25977e-07
Temperature range (K), min.	365.15
Temperature range (K), max.	440.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10588100&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1113
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1113.mol

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