

# Pentanoic acid, 2-methylpropyl ester

<b>Other names:</b>	2-METHYLPROPYL VALERATE 2-Methyl-1-propyl n-valerate ISOBUTYL PENTANOATE ISOBUTYL VALERINATE Isobutyl valerate Valeric acid, isobutyl ester
<b>Inchi:</b>	InChI=1S/C9H18O2/c1-4-5-6-9(10)11-7-8(2)3/h8H,4-7H2,1-3H3
<b>InchiKey:</b>	ADNADZOSMJDVIS-UHFFFAOYSA-N
<b>Formula:</b>	C9H18O2
<b>SMILES:</b>	CCCCC(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	158.24
<b>CAS:</b>	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	1027.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1009.00		NIST Webbook
rinpol	1009.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	1027.00		NIST Webbook
ripol	1253.00		NIST Webbook

ripol	1252.00		NIST Webbook
ripol	1252.00		NIST Webbook
tb	481.17	K	Joback Method
tc	658.49	K	Joback Method
tf	248.35	K	Joback Method
vc	0.557	m <sup>3</sup> /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	Paxs	248.35	Joback Method
dvisc	0.0020429	Paxs	287.15	Joback Method
dvisc	0.0010682	Paxs	325.96	Joback Method
dvisc	0.0006412	Paxs	364.76	Joback Method
dvisc	0.0004246	Paxs	403.56	Joback Method
dvisc	0.0003022	Paxs	442.37	Joback Method
dvisc	0.0002272	Paxs	481.17	Joback Method
hvapt	41.00	kJ/mol	293.00	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
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

<b>KDB Vapor Pressure Data:</b>	<a href="https://www.therc.org/research/kdb/hcprop/showprop.php?cmpid=1113">https://www.therc.org/research/kdb/hcprop/showprop.php?cmpid=1113</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>KDB:</b>	<a href="https://www.therc.org/files/research/kdb/mol/mol1113.mol">https://www.therc.org/files/research/kdb/mol/mol1113.mol</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C10588100&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C10588100&amp;Units=SI</a>

# Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfl:</b>	Liquid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rinpola:</b>	Non-polar retention indices
<b>ripola:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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