

# Pentanoic acid, 4-methyl, propyl ester

<b>Other names:</b>	Propyl isohexanoate
<b>Inchi:</b>	InChI=1S/C9H18O2/c1-4-7-11-9(10)6-5-8(2)3/h8H,4-7H2,1-3H3
<b>InchiKey:</b>	SDINNSBZSSSQXBH-UHFFFAOYSA-N
<b>Formula:</b>	C9H18O2
<b>SMILES:</b>	CCCOC(=O)CCC(C)C
<b>Mol. weight [g/mol]:</b>	158.24

## Physical Properties

Property code	Value	Unit	Source
gf	-211.46	kJ/mol	Joback Method
hf	-479.17	kJ/mol	Joback Method
hfus	18.33	kJ/mol	Joback Method
hvap	44.40	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.376		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	1038.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1035.00		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/molxK	569.83	Joback Method
cpg	374.44	J/molxK	599.38	Joback Method
cpg	386.04	J/molxK	628.93	Joback Method
cpg	397.15	J/molxK	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

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R34454&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R34454&amp;Units=SI</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>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<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>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<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>rinpol:</b>	Non-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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