

# Nonanoic acid, 1-methylethyl ester

<b>Other names:</b>	Isopropyl nonanoate isopropyl nonan-1-oate
<b>Inchi:</b>	InChI=1S/C12H24O2/c1-4-5-6-7-8-9-10-12(13)14-11(2)3/h11H,4-10H2,1-3H3
<b>InchiKey:</b>	DVFZGWDMFKTMFQ-UHFFFAOYSA-N
<b>Formula:</b>	C12H24O2
<b>SMILES:</b>	CCCCCCCCC(=O)OC(C)C
<b>Mol. weight [g/mol]:</b>	200.32
<b>CAS:</b>	28267-32-5

## Physical Properties

Property code	Value	Unit	Source
gf	-186.20	kJ/mol	Joback Method
hf	-541.09	kJ/mol	Joback Method
hfus	26.10	kJ/mol	Joback Method
hvap	51.07	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.689		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	1318.00		NIST Webbook
ripol	1516.00		NIST Webbook
tb	549.81	K	Joback Method
tc	722.69	K	Joback Method
tf	282.16	K	Joback Method
vc	0.726	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.44	J/molxK	549.81	Joback Method
cpg	480.46	J/molxK	578.62	Joback Method
cpg	495.83	J/molxK	607.44	Joback Method
cpg	510.57	J/molxK	636.25	Joback Method
cpg	524.69	J/molxK	665.07	Joback Method

cpg	538.20	J/mol×K	693.88	Joback Method
cpg	551.11	J/mol×K	722.69	Joback Method
dvisc	0.0042661	Paxs	282.16	Joback Method
dvisc	0.0017460	Paxs	326.77	Joback Method
dvisc	0.0008857	Paxs	371.38	Joback Method
dvisc	0.0005197	Paxs	415.99	Joback Method
dvisc	0.0003381	Paxs	460.59	Joback Method
dvisc	0.0002373	Paxs	505.20	Joback Method
dvisc	0.0001764	Paxs	549.81	Joback Method

## Sources

<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=C28267325&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C28267325&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>

## 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>ripol:</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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