

# Pentanoic acid, 2,2-dimethyl-, methyl ester

<b>Other names:</b>	Valeric acid, 2,2-dimethyl-, methyl ester Methyl «alpha», «alpha»-dimethylvalerate Methyl 2,2-dimethylvalerate 2,2-Dimethylvaleric acid, methyl ester
<b>Inchi:</b>	InChI=1S/C8H16O2/c1-5-6-8(2,3)7(9)10-4/h5-6H2,1-4H3
<b>InchiKey:</b>	QBIGLPZXHWTZKF-UHFFFAOYSA-N
<b>Formula:</b>	C8H16O2
<b>SMILES:</b>	CCCC(C)(C)C(=O)OC
<b>Mol. weight [g/mol]:</b>	144.21
<b>CAS:</b>	813-68-3

## Physical Properties

Property code	Value	Unit	Source
gf	-214.60	kJ/mol	Joback Method
hf	-462.00	kJ/mol	Joback Method
hfus	11.85	kJ/mol	Joback Method
hvap	41.26	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.986		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
tb	455.50	K	Joback Method
tc	641.54	K	Joback Method
tf	254.50	K	Joback Method
vc	0.496	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.32	J/molxK	455.50	Joback Method
cpg	295.73	J/molxK	486.51	Joback Method
cpg	308.53	J/molxK	517.51	Joback Method
cpg	320.73	J/molxK	548.52	Joback Method
cpg	332.35	J/molxK	579.53	Joback Method

cpg	343.41	J/mol×K	610.54	Joback Method
cpg	353.92	J/mol×K	641.54	Joback Method
dvisc	0.0046923	Paxs	254.50	Joback Method
dvisc	0.0021847	Paxs	288.00	Joback Method
dvisc	0.0011929	Paxs	321.50	Joback Method
dvisc	0.0007301	Paxs	355.00	Joback Method
dvisc	0.0004864	Paxs	388.50	Joback Method
dvisc	0.0003456	Paxs	422.00	Joback Method
dvisc	0.0002582	Paxs	455.50	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C813683&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C813683&amp;Units=SI</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>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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