

# Pentanoic acid, 2-methyl-, anhydride

<b>Inchi:</b>	InChI=1S/C12H22O3/c1-5-7-9(3)11(13)15-12(14)10(4)8-6-2/h9-10H,5-8H2,1-4H3
<b>InchiKey:</b>	NCYCWNILADFMPI-UHFFFAOYSA-N
<b>Formula:</b>	C12H22O3
<b>SMILES:</b>	CCCC(C)C(=O)OC(=O)C(C)CCC
<b>Mol. weight [g/mol]:</b>	214.30
<b>CAS:</b>	63169-61-9

## Physical Properties

Property code	Value	Unit	Source
gf	-317.56	kJ/mol	Joback Method
hf	-658.95	kJ/mol	Joback Method
hfus	24.18	kJ/mol	Joback Method
hvap	57.43	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.929		Crippen Method
mvol	188.950	ml/mol	McGowan Method
pc	1984.12	kPa	Joback Method
rinpol	1347.50		NIST Webbook
tb	603.24	K	Joback Method
tc	787.29	K	Joback Method
tf	317.09	K	Joback Method
vc	0.726	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.53	J/molxK	603.24	Joback Method
cpg	559.26	J/molxK	756.61	Joback Method
cpg	546.69	J/molxK	725.94	Joback Method
cpg	533.45	J/molxK	695.26	Joback Method
cpg	519.51	J/molxK	664.59	Joback Method
cpg	504.88	J/molxK	633.91	Joback Method
cpg	571.15	J/molxK	787.29	Joback Method
dvisc	0.0001688	Paxs	603.24	Joback Method

dvisc	0.0002286	Paxs	555.55	Joback Method
dvisc	0.0003276	Paxs	507.86	Joback Method
dvisc	0.0005061	Paxs	460.17	Joback Method
dvisc	0.0008644	Paxs	412.47	Joback Method
dvisc	0.0016982	Paxs	364.78	Joback Method
dvisc	0.0040877	Paxs	317.09	Joback Method

## Sources

<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=C63169619&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C63169619&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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