

# Pinonic acid

<b>Inchi:</b>	InChI=1S/C10H16O3/c1-6(11)8-4-7(5-9(12)13)10(8,2)3/h7-8H,4-5H2,1-3H3,(H,12,13)
<b>InchiKey:</b>	SIZDUQQDBXJXLQ-UHFFFAOYSA-N
<b>Formula:</b>	C10H16O3
<b>SMILES:</b>	CC(=O)C1CC(CC(=O)O)C1(C)C
<b>Mol. weight [g/mol]:</b>	184.23
<b>CAS:</b>	61826-55-9

## Physical Properties

Property code	Value	Unit	Source
chs	-5482.30	kJ/mol	NIST Webbook
gf	-333.60	kJ/mol	Joback Method
hf	-585.92	kJ/mol	Joback Method
hfs	-739.47	kJ/mol	NIST Webbook
hfus	20.82	kJ/mol	Joback Method
hvap	66.34	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.712		Crippen Method
mcvol	149.910	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
tb	630.03	K	Joback Method
tc	826.05	K	Joback Method
tf	392.98	K	Joback Method
vc	0.572	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.51	J/molxK	630.03	Joback Method
cpg	422.36	J/molxK	662.70	Joback Method
cpg	434.58	J/molxK	695.37	Joback Method
cpg	446.27	J/molxK	728.04	Joback Method
cpg	457.50	J/molxK	760.71	Joback Method
cpg	468.37	J/molxK	793.38	Joback Method
cpg	478.95	J/molxK	826.05	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=C61826559&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C61826559&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>

# Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfs:</b>	Solid 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>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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