

# 5-Dehydroquinic acid

<b>Inchi:</b>	InChI=1S/C7H10O6/c8-3-1-7(13,6(11)12)2-4(9)5(3)10/h3,5,8,10,13H,1-2H2,(H,11,12)
<b>InchiKey:</b>	WVMWZWGZRAXUBK-UHFFFAOYSA-N
<b>Formula:</b>	C7H10O6
<b>SMILES:</b>	O=C1CC(O)(C(=O)O)CC(O)C1O
<b>Mol. weight [g/mol]:</b>	190.15

## Physical Properties

Property code	Value	Unit	Source
gf	-787.19	kJ/mol	Joback Method
hf	-1018.13	kJ/mol	Joback Method
hfus	19.03	kJ/mol	Joback Method
hvap	107.55	kJ/mol	Joback Method
log10ws	0.85		Crippen Method
logp	-2.113		Crippen Method
mcvol	125.250	ml/mol	McGowan Method
pc	6503.64	kPa	Joback Method
tb	860.42	K	Joback Method
tc	1059.96	K	Joback Method
tf	552.88	K	Joback Method
vc	0.446	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.04	J/molxK	860.42	Joback Method
cpg	421.81	J/molxK	893.68	Joback Method
cpg	430.42	J/molxK	926.93	Joback Method
cpg	438.92	J/molxK	960.19	Joback Method
cpg	447.36	J/molxK	993.44	Joback Method
cpg	455.79	J/molxK	1026.70	Joback Method
cpg	464.28	J/molxK	1059.96	Joback Method

# Sources

<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=B6009879&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009879&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

# Legend

<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>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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