

# 2-Hydroxy-3-methoxyphenylacetonitrile

<b>Inchi:</b>	InChI=1S/C9H9NO2/c1-12-8-4-2-3-7(5-6-10)9(8)11/h2-4,11H,5H2,1H3
<b>InchiKey:</b>	HGPGOFBJMBBPAX-UHFFFAOYSA-N
<b>Formula:</b>	C9H9NO2
<b>SMILES:</b>	COc1cccc(CC#N)c1O
<b>Mol. weight [g/mol]:</b>	163.17
<b>CAS:</b>	42973-56-8

## Physical Properties

Property code	Value	Unit	Source
gf	1.24	kJ/mol	Joback Method
hf	-148.68	kJ/mol	Joback Method
hfus	21.20	kJ/mol	Joback Method
hvap	64.47	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.467		Crippen Method
mcvol	127.030	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
tb	642.10	K	Joback Method
tc	877.45	K	Joback Method
tf	429.07	K	Joback Method
vc	0.442	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.27	J/molxK	642.10	Joback Method
cpg	317.99	J/molxK	681.33	Joback Method
cpg	327.09	J/molxK	720.55	Joback Method
cpg	335.63	J/molxK	759.78	Joback Method
cpg	343.69	J/molxK	799.00	Joback Method
cpg	351.31	J/molxK	838.23	Joback Method
cpg	358.55	J/molxK	877.45	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=C42973568&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C42973568&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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