

# 3-Methoxy-4-nitrobenzoic acid

<b>Other names:</b>	Benzoic acid, 3-methoxy-4-nitro-
<b>Inchi:</b>	InChI=1S/C8H7NO5/c1-14-7-4-5(8(10)11)2-3-6(7)9(12)13/h2-4H,1H3,(H,10,11)
<b>InchiKey:</b>	PWURRRRGLCVBMX-UHFFFAOYSA-N
<b>Formula:</b>	C8H7NO5
<b>SMILES:</b>	COc1cc(C(=O)O)ccc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	197.14
<b>CAS:</b>	5081-36-7

## Physical Properties

Property code	Value	Unit	Source
gf	-225.56	kJ/mol	Joback Method
hf	-402.65	kJ/mol	Joback Method
hfus	27.98	kJ/mol	Joback Method
hsub	131.00 ± 1.10	kJ/mol	NIST Webbook
hvap	79.43	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.302		Crippen Method
mcvol	130.550	ml/mol	McGowan Method
pc	4244.08	kPa	Joback Method
tb	739.39	K	Joback Method
tc	966.92	K	Joback Method
tf	507.97	K	Joback Method
vc	0.500	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.61	J/mol×K	739.39	Joback Method
cpg	344.79	J/mol×K	777.31	Joback Method
cpg	352.32	J/mol×K	815.23	Joback Method
cpg	359.20	J/mol×K	853.16	Joback Method
cpg	365.43	J/mol×K	891.08	Joback Method
cpg	371.04	J/mol×K	929.00	Joback Method
cpg	376.02	J/mol×K	966.92	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=C5081367&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5081367&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>
<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>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<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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