

# 4-Methoxycarbonylbenzoic acid

Inchi:	InChI=1S/C9H8O4/c1-13-9(12)7-4-2-6(3-5-7)8(10)11/h2-5H,1H3,(H,10,11)
InchiKey:	REIDAMBAPLIATC-UHFFFAOYSA-N
Formula:	C9H8O4
SMILES:	COC(=O)c1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	180.16

## Physical Properties

Property code	Value	Unit	Source
gf	-371.98	kJ/mol	Joback Method
hf	-513.64	kJ/mol	Joback Method
hfus	21.19	kJ/mol	Joback Method
hvap	71.15	kJ/mol	Joback Method
log10ws	-2.97		Aqueous Solubility Prediction Method
logp	1.171		Crippen Method
mcvol	128.790	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method
tb	659.32	K	Joback Method
tc	868.49	K	Joback Method
tf	494.65	K	Aqueous Solubility Prediction Method
vc	0.480	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.39	J/molxK	659.32	Joback Method
cpg	322.42	J/molxK	694.18	Joback Method
cpg	330.85	J/molxK	729.04	Joback Method
cpg	338.71	J/molxK	763.90	Joback Method
cpg	346.00	J/molxK	798.77	Joback Method
cpg	352.72	J/molxK	833.63	Joback Method
cpg	358.88	J/molxK	868.49	Joback Method
dvisc	0.0015914	Paxs	413.04	Joback Method

dvisc	0.0007440	Paxs	454.09	Joback Method
dvisc	0.0003946	Paxs	495.13	Joback Method
dvisc	0.0002306	Paxs	536.18	Joback Method
dvisc	0.0001455	Paxs	577.23	Joback Method
dvisc	0.0000976	Paxs	618.27	Joback Method
dvisc	0.0000688	Paxs	659.32	Joback Method

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

## Legend

<b>cpg:</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>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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