

# 4-Mercaptobenzoic acid, S-methyl-, methyl ester

Other names:	4-CH3S-C6H4-COOCH3
Inchi:	InChI=1S/C9H10O2S/c1-11-9(10)7-3-5-8(12-2)6-4-7/h3-6H,1-2H3
InchiKey:	UQGNSVPCBCFZCE-UHFFFAOYSA-N
Formula:	C9H10O2S
SMILES:	COC(=O)c1ccc(SC)cc1
Mol. weight [g/mol]:	182.24
CAS:	3795-79-7

## Physical Properties

Property code	Value	Unit	Source
affp	864.30	kJ/mol	NIST Webbook
basg	833.30	kJ/mol	NIST Webbook
gf	-73.12	kJ/mol	Joback Method
hf	-206.96	kJ/mol	Joback Method
hfus	19.64	kJ/mol	Joback Method
hvap	54.54	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.195		Crippen Method
mcvol	137.700	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
rinpol	1580.70		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1580.70		NIST Webbook
rinpol	1578.00		NIST Webbook
rinpol	1610.00		NIST Webbook
tb	582.05	K	Joback Method
tc	819.33	K	Joback Method
tf	336.69	K	Joback Method
vc	0.509	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.44	J/molxK	582.05	Joback Method

cpg	315.94	J/mol×K	621.60	Joback Method
cpg	327.66	J/mol×K	661.14	Joback Method
cpg	338.59	J/mol×K	700.69	Joback Method
cpg	348.75	J/mol×K	740.23	Joback Method
cpg	358.12	J/mol×K	779.78	Joback Method
cpg	366.72	J/mol×K	819.33	Joback Method

## Sources

<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=C3795797&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3795797&amp;Units=SI</a>

## Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<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>rinpol:</b>	Non-polar retention indices
<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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