

# Benzoic acid, 3-(methylthio)-, ethyl ester

<b>Inchi:</b>	InChI=1S/C10H12O2S/c1-3-12-10(11)8-5-4-6-9(7-8)13-2/h4-7H,3H2,1-2H3
<b>InchiKey:</b>	DXATWXQPWLCGPA-UHFFFAOYSA-N
<b>Formula:</b>	C10H12O2S
<b>SMILES:</b>	CCOC(=O)c1cccc(SC)c1
<b>Mol. weight [g/mol]:</b>	196.27

## Physical Properties

Property code	Value	Unit	Source
gf	-64.70	kJ/mol	Joback Method
hf	-227.60	kJ/mol	Joback Method
hfus	22.23	kJ/mol	Joback Method
hvap	56.77	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.585		Crippen Method
mcvol	151.790	ml/mol	McGowan Method
pc	3089.85	kPa	Joback Method
rinpol	1607.00		NIST Webbook
rinpol	1607.00		NIST Webbook
tb	604.93	K	Joback Method
tc	837.42	K	Joback Method
tf	347.96	K	Joback Method
vc	0.566	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.05	J/mol×K	604.93	Joback Method
cpg	363.45	J/mol×K	643.68	Joback Method
cpg	376.01	J/mol×K	682.43	Joback Method
cpg	387.72	J/mol×K	721.18	Joback Method
cpg	398.60	J/mol×K	759.92	Joback Method
cpg	408.65	J/mol×K	798.67	Joback Method
cpg	417.88	J/mol×K	837.42	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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=U374957&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U374957&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hvp:</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>rinp:</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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