

# Benzoic acid, 2-(methylthio)-, propyl ester

<b>Inchi:</b>	InChI=1S/C11H14O2S/c1-3-8-13-11(12)9-6-4-5-7-10(9)14-2/h4-7H,3,8H2,1-2H3
<b>InchiKey:</b>	HDZTYNJKAIBYQU-UHFFFAOYSA-N
<b>Formula:</b>	C11H14O2S
<b>SMILES:</b>	CCCOC(=O)c1ccccc1SC
<b>Mol. weight [g/mol]:</b>	210.29

## Physical Properties

Property code	Value	Unit	Source
gf	-56.28	kJ/mol	Joback Method
hf	-248.24	kJ/mol	Joback Method
hfus	24.82	kJ/mol	Joback Method
hvap	58.99	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.975		Crippen Method
mcvol	165.880	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
rinsol	1714.00		NIST Webbook
tb	627.81	K	Joback Method
tc	855.76	K	Joback Method
tf	359.23	K	Joback Method
vc	0.622	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.30	J/mol×K	627.81	Joback Method
cpg	412.46	J/mol×K	665.80	Joback Method
cpg	425.72	J/mol×K	703.79	Joback Method
cpg	438.10	J/mol×K	741.78	Joback Method
cpg	449.59	J/mol×K	779.77	Joback Method
cpg	460.21	J/mol×K	817.77	Joback Method
cpg	469.97	J/mol×K	855.76	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U374954&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U374954&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>
<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>

# 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>rinpola:</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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