

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

Inchi:	InChI=1S/C12H16O2S/c1-9(2)8-14-12(13)10-6-4-5-7-11(10)15-3/h4-7,9H,8H2,1-3H3
InchiKey:	BNMBRPQKSQQNIW-UHFFFAOYSA-N
Formula:	C12H16O2S
SMILES:	CSc1ccccc1C(=O)OCC(C)C
Mol. weight [g/mol]:	224.32

## Physical Properties

Property code	Value	Unit	Source
gf	-50.30	kJ/mol	Joback Method
hf	-274.16	kJ/mol	Joback Method
hfus	23.88	kJ/mol	Joback Method
hvap	60.83	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.221		Crippen Method
mcvol	179.970	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
rinpol	1769.00		NIST Webbook
rinpol	1769.00		NIST Webbook
tb	650.25	K	Joback Method
tc	878.49	K	Joback Method
tf	355.50	K	Joback Method
vc	0.671	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.59	J/mol×K	650.25	Joback Method
cpg	463.72	J/mol×K	688.29	Joback Method
cpg	477.86	J/mol×K	726.33	Joback Method
cpg	491.02	J/mol×K	764.37	Joback Method
cpg	503.21	J/mol×K	802.41	Joback Method
cpg	514.45	J/mol×K	840.45	Joback Method
cpg	524.75	J/mol×K	878.49	Joback Method

# Sources

<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=U375376&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U375376&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>
<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>

# 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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