

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

Inchi:	InChI=1S/C13H18O2S/c1-10(2)7-8-15-13(14)11-5-4-6-12(9-11)16-3/h4-6,9-10H,7-8H2,1
InchiKey:	HZH ZKPNBFCNQSI-UHFFFAOYSA-N
Formula:	C13H18O2S
SMILES:	CSc1cccc(C(=O)OCCC(C)C)c1
Mol. weight [g/mol]:	238.35

## Physical Properties

Property code	Value	Unit	Source
gf	-41.88	kJ/mol	Joback Method
hf	-294.80	kJ/mol	Joback Method
hfus	26.47	kJ/mol	Joback Method
hvap	63.06	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.611		Crippen Method
mcvol	194.060	ml/mol	McGowan Method
pc	2313.61	kPa	Joback Method
rinqol	1878.00		NIST Webbook
tb	673.13	K	Joback Method
tc	897.16	K	Joback Method
tf	366.77	K	Joback Method
vc	0.728	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.83	J/molxK	673.13	Joback Method
cpg	515.48	J/molxK	710.47	Joback Method
cpg	530.10	J/molxK	747.81	Joback Method
cpg	543.70	J/molxK	785.14	Joback Method
cpg	556.31	J/molxK	822.48	Joback Method
cpg	567.93	J/molxK	859.82	Joback Method
cpg	578.59	J/molxK	897.16	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U375365&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U375365&amp;Units=SI</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>h vap:</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>m cvol:</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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