

# Benzoic acid, 4-(isopropylthio)-, isopropyl ester

Inchi:	InChI=1S/C13H18O2S/c1-9(2)15-13(14)11-5-7-12(8-6-11)16-10(3)4/h5-10H,1-4H3
InchiKey:	CVSBRDUPDMNVGA-UHFFFAOYSA-N
Formula:	C13H18O2S
SMILES:	CC(C)OC(=O)c1ccc(SC(C)C)cc1
Mol. weight [g/mol]:	238.35

## Physical Properties

Property code	Value	Unit	Source
gf	-44.32	kJ/mol	Joback Method
hf	-300.08	kJ/mol	Joback Method
hfus	22.95	kJ/mol	Joback Method
hvap	62.67	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.752		Crippen Method
mcvol	194.060	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
rinqol	1757.00		NIST Webbook
tb	672.69	K	Joback Method
tc	901.16	K	Joback Method
tf	351.77	K	Joback Method
vc	0.722	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.34	J/mol×K	672.69	Joback Method
cpg	516.33	J/mol×K	710.77	Joback Method
cpg	531.24	J/mol×K	748.85	Joback Method
cpg	545.08	J/mol×K	786.92	Joback Method
cpg	557.87	J/mol×K	825.00	Joback Method
cpg	569.62	J/mol×K	863.08	Joback Method
cpg	580.37	J/mol×K	901.16	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=U375406&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U375406&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>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>mccvol:</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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