

# isobutyl 3-(methylthio)propanoate

<b>Inchi:</b>	InChI=1S/C8H16O2S/c1-7(2)6-10-8(9)4-5-11-3/h7H,4-6H2,1-3H3
<b>InchiKey:</b>	TUEGKTDHUCFRQP-UHFFFAOYSA-N
<b>Formula:</b>	C8H16O2S
<b>SMILES:</b>	CSCCC(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	176.28

## Physical Properties

Property code	Value	Unit	Source
gf	-186.76	kJ/mol	Joback Method
hf	-416.66	kJ/mol	Joback Method
hfus	19.87	kJ/mol	Joback Method
hvap	48.99	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.939		Crippen Method
mcvol	147.370	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
ripol	1681.00		NIST Webbook
tb	527.07	K	Joback Method
tc	725.43	K	Joback Method
tf	271.48	K	Joback Method
vc	0.555	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.94	J/mol×K	527.07	Joback Method
cpg	345.16	J/mol×K	560.13	Joback Method
cpg	357.82	J/mol×K	593.19	Joback Method
cpg	369.91	J/mol×K	626.25	Joback Method
cpg	381.43	J/mol×K	659.31	Joback Method
cpg	392.38	J/mol×K	692.37	Joback Method
cpg	402.77	J/mol×K	725.43	Joback Method

# Sources

<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=R327316&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R327316&amp;Units=SI</a>
<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>

# 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>ripol:</b>	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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