

# bis(1-methyl-2-oxopropyl) sulfide

<b>Inchi:</b>	InChI=1S/C8H14O2S/c1-5(9)7(3)11-8(4)6(2)10/h7-8H,1-4H3
<b>InchiKey:</b>	YGVGCMGLHWUOCP-UHFFFAOYSA-N
<b>Formula:</b>	C8H14O2S
<b>SMILES:</b>	CC(=O)C(C)SC(C)C(C)=O
<b>Mol. weight [g/mol]:</b>	174.26

## Physical Properties

Property code	Value	Unit	Source
gf	-213.12	kJ/mol	Joback Method
hf	-402.30	kJ/mol	Joback Method
hfus	16.76	kJ/mol	Joback Method
hvap	52.94	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.675		Crippen Method
mcvol	143.070	ml/mol	McGowan Method
pc	2995.87	kPa	Joback Method
rinpol	1359.00		NIST Webbook
tb	558.08	K	Joback Method
tc	771.32	K	Joback Method
tf	284.18	K	Joback Method
vc	0.537	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.61	J/molxK	558.08	Joback Method
cpg	338.38	J/molxK	593.62	Joback Method
cpg	350.46	J/molxK	629.16	Joback Method
cpg	361.86	J/molxK	664.70	Joback Method
cpg	372.59	J/molxK	700.24	Joback Method
cpg	382.66	J/molxK	735.78	Joback Method
cpg	392.08	J/molxK	771.32	Joback Method

# Sources

<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>
<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=R223120&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R223120&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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