

# 3-(1-Methyl-2-oxobutylidithio)pentan-2-one, #1

<b>Inchi:</b>	InChI=1S/C10H18O2S2/c1-5-9(12)8(4)13-14-10(6-2)7(3)11/h8,10H,5-6H2,1-4H3
<b>InchiKey:</b>	XXXOWSFREAVVBG-UHFFFAOYSA-N
<b>Formula:</b>	C10H18O2S2
<b>SMILES:</b>	CCC(=O)C(C)SSC(CC)C(C)=O
<b>Mol. weight [g/mol]:</b>	234.38

## Physical Properties

Property code	Value	Unit	Source
gf	-163.16	kJ/mol	Joback Method
hf	-401.71	kJ/mol	Joback Method
hfus	26.07	kJ/mol	Joback Method
hvap	64.20	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.103		Crippen Method
mcvol	187.600	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	1624.00		NIST Webbook
rinpol	1624.00		NIST Webbook
tb	672.62	K	Joback Method
tc	895.13	K	Joback Method
tf	341.12	K	Joback Method
vc	0.704	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.93	J/mol×K	672.62	Joback Method
cpg	488.07	J/mol×K	709.70	Joback Method
cpg	501.29	J/mol×K	746.79	Joback Method
cpg	513.59	J/mol×K	783.87	Joback Method
cpg	524.98	J/mol×K	820.96	Joback Method
cpg	535.47	J/mol×K	858.04	Joback Method
cpg	545.08	J/mol×K	895.13	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=R90541&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R90541&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r in pol:</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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