

# 3-[(1-methyl-2-oxobuty1)-trithio]-2-pentanone

<b>Inchi:</b>	InChI=1S/C10H18O2S3/c1-5-9(12)8(4)13-15-14-10(6-2)7(3)11/h8,10H,5-6H2,1-4H3
<b>InchiKey:</b>	FIWVYTBRDVZKHN-UHFFFAOYSA-N
<b>Formula:</b>	C10H18O2S3
<b>SMILES:</b>	CCC(=O)C(C)SSSC(CC)C(C)=O
<b>Mol. weight [g/mol]:</b>	266.44

## Physical Properties

Property code	Value	Unit	Source
gf	-130.04	kJ/mol	Joback Method
hf	-359.84	kJ/mol	Joback Method
hfus	30.20	kJ/mol	Joback Method
hvap	71.02	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.751		Crippen Method
mcvol	203.950	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinpol	1888.00		NIST Webbook
tb	741.40	K	Joback Method
tc	978.92	K	Joback Method
tf	375.52	K	Joback Method
vc	0.757	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.71	J/molxK	741.40	Joback Method
cpg	539.25	J/molxK	780.99	Joback Method
cpg	551.68	J/molxK	820.57	Joback Method
cpg	562.99	J/molxK	860.16	Joback Method
cpg	573.20	J/molxK	899.74	Joback Method
cpg	582.31	J/molxK	939.33	Joback Method
cpg	590.31	J/molxK	978.92	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=R223046&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R223046&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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