

# 2-[(1-methyl-2-oxopropyl)-dithio]-3-pentanone

<b>Inchi:</b>	InChI=1S/C9H16O2S2/c1-5-9(11)8(4)13-12-7(3)6(2)10/h7-8H,5H2,1-4H3
<b>InchiKey:</b>	DYAXZUZAGRJLCX-UHFFFAOYSA-N
<b>Formula:</b>	C9H16O2S2
<b>SMILES:</b>	CCC(=O)C(C)SSC(C)C(C)=O
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	-171.58	kJ/mol	Joback Method
hf	-381.07	kJ/mol	Joback Method
hfus	23.48	kJ/mol	Joback Method
hvap	61.98	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.713		Crippen Method
mcvol	173.510	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
rinpol	1567.00		NIST Webbook
rinpol	1562.00		NIST Webbook
rinpol	1562.00		NIST Webbook
tb	649.74	K	Joback Method
tc	876.37	K	Joback Method
tf	329.85	K	Joback Method
vc	0.647	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.62	J/molxK	649.74	Joback Method
cpg	437.16	J/molxK	687.51	Joback Method
cpg	449.82	J/molxK	725.28	Joback Method
cpg	461.60	J/molxK	763.05	Joback Method
cpg	472.51	J/molxK	800.83	Joback Method
cpg	482.56	J/molxK	838.60	Joback Method
cpg	491.75	J/molxK	876.37	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=R222934&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R222934&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>hvp:</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>rlnol:</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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