

# 3-methyl-4,6-dithianonane

<b>Inchi:</b>	InChI=1S/C8H18S2/c1-4-6-9-7-10-8(3)5-2/h8H,4-7H2,1-3H3
<b>InchiKey:</b>	ZKEDAGLBUZZGBW-UHFFFAOYSA-N
<b>Formula:</b>	C8H18S2
<b>SMILES:</b>	CCCSCSC(C)CC
<b>Mol. weight [g/mol]:</b>	178.36

## Physical Properties

Property code	Value	Unit	Source
gf	80.28	kJ/mol	Joback Method
hf	-129.99	kJ/mol	Joback Method
hfus	21.21	kJ/mol	Joback Method
hvap	46.65	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.619		Crippen Method
mcvol	156.280	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
rinqol	1278.00		NIST Webbook
tb	519.56	K	Joback Method
tc	730.16	K	Joback Method
tf	233.72	K	Joback Method
vc	0.586	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.00	J/mol×K	519.56	Joback Method
cpg	355.88	J/mol×K	554.66	Joback Method
cpg	370.06	J/mol×K	589.76	Joback Method
cpg	383.53	J/mol×K	624.86	Joback Method
cpg	396.31	J/mol×K	659.96	Joback Method
cpg	408.41	J/mol×K	695.06	Joback Method
cpg	419.83	J/mol×K	730.16	Joback Method

# Sources

<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=R156728&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R156728&amp;Units=SI</a>
<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>

# 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>rinpola:</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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