

# 3,3-dimethyl-4-thianonane

<b>Inchi:</b>	InChI=1S/C10H22S/c1-5-7-8-9-11-10(3,4)6-2/h5-9H2,1-4H3
<b>InchiKey:</b>	UAUQTCCDDTCHXRU-UHFFFAOYSA-N
<b>Formula:</b>	C10H22S
<b>SMILES:</b>	CCCCCSC(C)(C)CC
<b>Mol. weight [g/mol]:</b>	174.35

## Physical Properties

Property code	Value	Unit	Source
gf	69.28	kJ/mol	Joback Method
hf	-216.61	kJ/mol	Joback Method
hfus	18.37	kJ/mol	Joback Method
hvap	43.38	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	4.098		Crippen Method
mcvol	168.110	ml/mol	McGowan Method
pc	2179.52	kPa	Joback Method
rinpol	1189.00		NIST Webbook
tb	493.75	K	Joback Method
tc	686.87	K	Joback Method
tf	239.28	K	Joback Method
vc	0.638	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.65	J/mol×K	493.75	Joback Method
cpg	395.65	J/mol×K	525.94	Joback Method
cpg	411.80	J/mol×K	558.12	Joback Method
cpg	427.12	J/mol×K	590.31	Joback Method
cpg	441.65	J/mol×K	622.50	Joback Method
cpg	455.41	J/mol×K	654.69	Joback Method
cpg	468.45	J/mol×K	686.87	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=R296301&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R296301&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>
<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>

# 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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