

# 2,8-dimethyl-4,6-dithianonane

<b>Inchi:</b>	InChI=1S/C9H20S2/c1-8(2)5-10-7-11-6-9(3)4/h8-9H,5-7H2,1-4H3
<b>InchiKey:</b>	JJMNQJWIFSUMOL-UHFFFAOYSA-N
<b>Formula:</b>	C9H20S2
<b>SMILES:</b>	CC(C)CSCSCC(C)C
<b>Mol. weight [g/mol]:</b>	192.38

## Physical Properties

Property code	Value	Unit	Source
gf	86.26	kJ/mol	Joback Method
hf	-155.91	kJ/mol	Joback Method
hfus	20.28	kJ/mol	Joback Method
hvap	48.49	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.722		Crippen Method
mcvol	170.370	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinsol	1329.00		NIST Webbook
tb	542.00	K	Joback Method
tc	753.86	K	Joback Method
tf	229.99	K	Joback Method
vc	0.635	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.59	J/mol×K	542.00	Joback Method
cpg	403.78	J/mol×K	577.31	Joback Method
cpg	419.15	J/mol×K	612.62	Joback Method
cpg	433.73	J/mol×K	647.93	Joback Method
cpg	447.52	J/mol×K	683.24	Joback Method
cpg	460.55	J/mol×K	718.55	Joback Method
cpg	472.80	J/mol×K	753.86	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=R155958&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R155958&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>

# 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>hvac:</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>mccol:</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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