

# 2,4,5,6-Tetrathianonane, 3-ethyl

<b>Inchi:</b>	InChI=1S/C7H16S4/c1-4-6-9-11-10-7(5-2)8-3/h7H,4-6H2,1-3H3
<b>InchiKey:</b>	BKTPSJHQEKQRAY-UHFFFAOYSA-N
<b>Formula:</b>	C7H16S4
<b>SMILES:</b>	CCSSSSC(CC)SC
<b>Mol. weight [g/mol]:</b>	228.46

## Physical Properties

Property code	Value	Unit	Source
gf	138.10	kJ/mol	Joback Method
hf	-25.61	kJ/mol	Joback Method
hfus	26.88	kJ/mol	Joback Method
hvap	58.06	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.525		Crippen Method
mcvol	174.890	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
rinpol	1627.00		NIST Webbook
tb	634.24	K	Joback Method
tc	887.39	K	Joback Method
tf	291.25	K	Joback Method
vc	0.637	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.86	J/mol×K	634.24	Joback Method
cpg	411.25	J/mol×K	676.43	Joback Method
cpg	424.64	J/mol×K	718.62	Joback Method
cpg	437.03	J/mol×K	760.81	Joback Method
cpg	448.39	J/mol×K	803.01	Joback Method
cpg	458.71	J/mol×K	845.20	Joback Method
cpg	467.97	J/mol×K	887.39	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=R56820&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R56820&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>mccvol:</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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