

# 6-methyl-4,5-dithia-1-octene

<b>Inchi:</b>	InChI=1S/C7H14S2/c1-4-6-8-9-7(3)5-2/h4,7H,1,5-6H2,2-3H3
<b>InchiKey:</b>	CVNONOJAARHURZ-UHFFFAOYSA-N
<b>Formula:</b>	C7H14S2
<b>SMILES:</b>	C=CCSSC(C)CC
<b>Mol. weight [g/mol]:</b>	162.32

## Physical Properties

Property code	Value	Unit	Source
gf	159.70	kJ/mol	Joback Method
hf	16.08	kJ/mol	Joback Method
hfus	17.34	kJ/mol	Joback Method
hvap	43.75	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.352		Crippen Method
mcvol	137.890	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
rinsol	1152.00		NIST Webbook
tb	493.36	K	Joback Method
tc	712.09	K	Joback Method
tf	220.69	K	Joback Method
vc	0.510	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.92	J/mol×K	493.36	Joback Method
cpg	292.06	J/mol×K	529.82	Joback Method
cpg	304.53	J/mol×K	566.27	Joback Method
cpg	316.35	J/mol×K	602.73	Joback Method
cpg	327.54	J/mol×K	639.18	Joback Method
cpg	338.08	J/mol×K	675.64	Joback Method
cpg	348.01	J/mol×K	712.09	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=R157598&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R157598&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>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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