

# 4,7-dithia-1-octene

<b>Inchi:</b>	InChI=1S/C6H12S2/c1-3-4-8-6-5-7-2/h3H,1,4-6H2,2H3
<b>InchiKey:</b>	KYQJVWSAHLHJPF-UHFFFAOYSA-N
<b>Formula:</b>	C6H12S2
<b>SMILES:</b>	C=CCSCCSC
<b>Mol. weight [g/mol]:</b>	148.29

## Physical Properties

Property code	Value	Unit	Source
gf	153.72	kJ/mol	Joback Method
hf	42.00	kJ/mol	Joback Method
hfus	18.28	kJ/mol	Joback Method
hvap	41.91	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	2.269		Crippen Method
mcvol	123.800	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
rinpol	1179.00		NIST Webbook
rinpol	1179.00		NIST Webbook
tb	470.92	K	Joback Method
tc	687.95	K	Joback Method
tf	224.42	K	Joback Method
vc	0.461	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.15	J/mol×K	470.92	Joback Method
cpg	248.69	J/mol×K	507.09	Joback Method
cpg	259.67	J/mol×K	543.26	Joback Method
cpg	270.11	J/mol×K	579.43	Joback Method
cpg	280.01	J/mol×K	615.61	Joback Method
cpg	289.38	J/mol×K	651.78	Joback Method
cpg	298.22	J/mol×K	687.95	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<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=R157078&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R157078&amp;Units=SI</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>hvp:</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>rinp:</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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