

# 3-Ethyl-1,2-dithi-4-ene

<b>Inchi:</b>	InChI=1S/C6H10S2/c1-2-6-4-3-5-7-8-6/h3-4,6H,2,5H2,1H3
<b>InchiKey:</b>	QRXGPSRNGFYLIU-UHFFFAOYSA-N
<b>Formula:</b>	C6H10S2
<b>SMILES:</b>	CCC1C=CCSS1
<b>Mol. weight [g/mol]:</b>	146.27

## Physical Properties

Property code	Value	Unit	Source
gf	133.77	kJ/mol	Joback Method
hf	35.45	kJ/mol	Joback Method
hfus	11.67	kJ/mol	Joback Method
hvap	41.30	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.716		Crippen Method
mcvol	112.940	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method
rinsol	1113.00		NIST Webbook
tb	451.05	K	Joback Method
tc	692.78	K	Joback Method
tf	332.42	K	Joback Method
vc	0.383	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.23	J/mol×K	451.05	Joback Method
cpg	224.13	J/mol×K	491.34	Joback Method
cpg	237.14	J/mol×K	531.63	Joback Method
cpg	249.31	J/mol×K	571.91	Joback Method
cpg	260.65	J/mol×K	612.20	Joback Method
cpg	271.22	J/mol×K	652.49	Joback Method
cpg	281.04	J/mol×K	692.78	Joback Method

# Sources

<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=R261380&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R261380&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>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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