

# 4-Ethyl-2,3,5-trithia-6-octene

<b>Inchi:</b>	InChI=1S/C7H14S3/c1-4-6-9-7(5-2)10-8-3/h4,6-7H,5H2,1-3H3/b6-4+
<b>InchiKey:</b>	MLJHEPZOIZWECF-GQCTYLIASA-N
<b>Formula:</b>	C7H14S3
<b>SMILES:</b>	CC=CSC(CC)SSC
<b>Mol. weight [g/mol]:</b>	194.38
<b>CAS:</b>	126876-23-1

## Physical Properties

Property code	Value	Unit	Source
gf	185.20	kJ/mol	Joback Method
hf	49.74	kJ/mol	Joback Method
hfus	22.95	kJ/mol	Joback Method
hvap	51.20	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.001		Crippen Method
mcvol	154.240	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
rinpol	1407.00		NIST Webbook
rinpol	1390.60		NIST Webbook
rinpol	1436.50		NIST Webbook
rinpol	1436.50		NIST Webbook
rinpol	1407.00		NIST Webbook
rinpol	1390.60		NIST Webbook
tb	569.62	K	Joback Method
tc	815.04	K	Joback Method
tf	251.77	K	Joback Method
vc	0.564	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.38	J/mol×K	569.62	Joback Method
cpg	341.05	J/mol×K	610.52	Joback Method
cpg	353.85	J/mol×K	651.43	Joback Method

cpg	365.81	J/mol×K	692.33	Joback Method
cpg	376.94	J/mol×K	733.24	Joback Method
cpg	387.26	J/mol×K	774.14	Joback Method
cpg	396.77	J/mol×K	815.04	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=C126876231&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C126876231&amp;Units=SI</a>
<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>

## 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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</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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