

# 1-Oxa-4,7,10-trithiacyclododecane

<b>Inchi:</b>	InChI=1S/C8H16OS3/c1-3-10-5-7-12-8-6-11-4-2-9-1/h1-8H2
<b>InchiKey:</b>	GBFAGTGBGJQKBG-UHFFFAOYSA-N
<b>Formula:</b>	C8H16OS3
<b>SMILES:</b>	C1CSCCSCCSCCO1
<b>Mol. weight [g/mol]:</b>	224.41

## Physical Properties

Property code	Value	Unit	Source
gf	9.50	kJ/mol	Joback Method
hf	-166.97	kJ/mol	Joback Method
hfus	13.59	kJ/mol	Joback Method
hvap	57.12	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	2.216		Crippen Method
mcvol	167.640	ml/mol	McGowan Method
pc	3786.98	kPa	Joback Method
rinpol	1885.00		NIST Webbook
rinpol	1885.00		NIST Webbook
tb	602.72	K	Joback Method
tc	903.58	K	Joback Method
tf	447.34	K	Joback Method
vc	0.528	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.65	J/mol×K	602.72	Joback Method
cpg	416.55	J/mol×K	652.86	Joback Method
cpg	437.48	J/mol×K	703.01	Joback Method
cpg	456.43	J/mol×K	753.15	Joback Method
cpg	473.35	J/mol×K	803.29	Joback Method
cpg	488.22	J/mol×K	853.43	Joback Method
cpg	501.02	J/mol×K	903.58	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=R41459&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R41459&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>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>rlnol:</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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