

# 2,4,6-Trithiaheptane

<b>Inchi:</b>	InChI=1S/C4H10S3/c1-5-3-7-4-6-2/h3-4H2,1-2H3
<b>InchiKey:</b>	PQFOEUXAUYRCAY-UHFFFAOYSA-N
<b>Formula:</b>	C4H10S3
<b>SMILES:</b>	CSCSCSC
<b>Mol. weight [g/mol]:</b>	154.32

## Physical Properties

Property code	Value	Unit	Source
gf	82.16	kJ/mol	Joback Method
hf	-0.28	kJ/mol	Joback Method
hfus	18.51	kJ/mol	Joback Method
hvap	44.95	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.361		Crippen Method
mcvol	116.270	ml/mol	McGowan Method
pc	4156.97	kPa	Joback Method
rinqol	1242.00		NIST Webbook
tb	497.26	K	Joback Method
tc	740.19	K	Joback Method
tf	238.04	K	Joback Method
vc	0.421	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.75	J/mol×K	497.26	Joback Method
cpg	227.03	J/mol×K	537.75	Joback Method
cpg	236.83	J/mol×K	578.24	Joback Method
cpg	246.12	J/mol×K	618.73	Joback Method
cpg	254.89	J/mol×K	659.22	Joback Method
cpg	263.12	J/mol×K	699.70	Joback Method
cpg	270.79	J/mol×K	740.19	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R587201&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R587201&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>
<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>

# 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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