

# Heptanethioic acid, S-methyl ester

<b>Other names:</b>	S-Methyl thioheptanoate
<b>Inchi:</b>	InChI=1S/C8H16OS/c1-3-4-5-6-7-8(9)10-2/h3-7H2,1-2H3
<b>InchiKey:</b>	XBNCUVKYQNARCE-UHFFFAOYSA-N
<b>Formula:</b>	C8H16OS
<b>SMILES:</b>	CCCCCCC(=O)SC
<b>Mol. weight [g/mol]:</b>	160.28
<b>CAS:</b>	2432-82-8

## Physical Properties

Property code	Value	Unit	Source
gf	-79.32	kJ/mol	Joback Method
hf	-279.16	kJ/mol	Joback Method
hfus	22.20	kJ/mol	Joback Method
hvap	46.97	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.846		Crippen Method
mcvol	141.500	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
ripol	1666.00		NIST Webbook
ripol	1666.00		NIST Webbook
tb	505.09	K	Joback Method
tc	700.77	K	Joback Method
tf	264.25	K	Joback Method
vc	0.543	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.58	J/molxK	505.09	Joback Method
cpg	320.67	J/molxK	537.70	Joback Method
cpg	333.17	J/molxK	570.32	Joback Method
cpg	345.09	J/molxK	602.93	Joback Method
cpg	356.44	J/molxK	635.54	Joback Method
cpg	367.24	J/molxK	668.15	Joback Method

## Sources

<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=C2432828&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2432828&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>

## 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>ripol:</b>	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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