

# CH<sub>2</sub>=C(CH<sub>3</sub>)-SCH<sub>3</sub>

Inchi:	InChI=1S/C4H8S/c1-4(2)5-3/h1H2,2-3H3
InchiKey:	ITKBWZPRAFZVNW-UHFFFAOYSA-N
Formula:	C4H8S
SMILES:	C=C(C)SC
Mol. weight [g/mol]:	88.17
CAS:	7594-44-7

## Physical Properties

Property code	Value	Unit	Source
affp	888.60	kJ/mol	NIST Webbook
basg	859.70	kJ/mol	NIST Webbook
gf	95.21	kJ/mol	Joback Method
hf	31.62	kJ/mol	Joback Method
hfus	7.66	kJ/mol	Joback Method
hvap	30.73	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.883		Crippen Method
mcvol	79.270	ml/mol	McGowan Method
pc	4227.54	kPa	Joback Method
tb	356.26	K	Joback Method
tc	555.87	K	Joback Method
tf	153.52	K	Joback Method
vc	0.295	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	122.33	J/mol×K	356.26	Joback Method
cpg	130.20	J/mol×K	389.53	Joback Method
cpg	137.74	J/mol×K	422.80	Joback Method
cpg	144.97	J/mol×K	456.06	Joback Method
cpg	151.88	J/mol×K	489.33	Joback Method
cpg	158.49	J/mol×K	522.60	Joback Method
cpg	164.80	J/mol×K	555.87	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=C7594447&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7594447&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>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<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>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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