

# 4-Hepten-3-one, 1,1,2,2-tetrafluoro-5-mercapto-

Inchi:	InChI=1S/C7H8F4OS/c1-2-4(13)3-5(12)7(10,11)6(8)9/h3,6,13H,2H2,1H3/b4-3-
InchiKey:	CECUBSXYFQYELM-ARJAWSKDSA-N
Formula:	C7H8F4OS
SMILES:	CCC(S)=CC(=O)C(F)(F)C(F)F
Mol. weight [g/mol]:	216.20
CAS:	88552-05-0

## Physical Properties

Property code	Value	Unit	Source
gf	-798.64	kJ/mol	Joback Method
hf	-952.95	kJ/mol	Joback Method
hfus	19.80	kJ/mol	Joback Method
hvap	39.75	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.680		Crippen Method
mvol	130.190	ml/mol	McGowan Method
pc	2893.62	kPa	Joback Method
tb	473.74	K	Joback Method
tc	660.95	K	Joback Method
tf	225.78	K	Joback Method
vc	0.523	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.04	J/mol×K	473.74	Joback Method
cpg	292.84	J/mol×K	504.94	Joback Method
cpg	302.93	J/mol×K	536.14	Joback Method
cpg	312.35	J/mol×K	567.34	Joback Method
cpg	321.12	J/mol×K	598.54	Joback Method
cpg	329.30	J/mol×K	629.74	Joback Method
cpg	336.92	J/mol×K	660.95	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=C88552050&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C88552050&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>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>hvac:</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>mccol:</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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