

# 3-Hexene-2-thione,5,5,6,6-tetrafluoro-4-hydroxy-

<b>Inchi:</b>	InChI=1S/C6H6F4OS/c1-3(12)2-4(11)6(9,10)5(7)8/h2,5,11H,1H3/b4-2-
<b>InchiKey:</b>	GJTXQUBCEARLFL-RQOWECAXSA-N
<b>Formula:</b>	C6H6F4OS
<b>SMILES:</b>	CC(=S)C=C(O)C(F)(F)C(F)F
<b>Mol. weight [g/mol]:</b>	202.17
<b>CAS:</b>	88551-98-8

## Physical Properties

Property code	Value	Unit	Source
gf	-727.29	kJ/mol	Joback Method
hf	-863.94	kJ/mol	Joback Method
hfus	20.26	kJ/mol	Joback Method
hvap	47.44	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.719		Crippen Method
mcvol	116.100	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
tb	496.35	K	Joback Method
tc	671.48	K	Joback Method
tf	223.21	K	Joback Method
vc	0.463	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.60	J/molxK	496.35	Joback Method
cpg	265.60	J/molxK	525.54	Joback Method
cpg	272.98	J/molxK	554.73	Joback Method
cpg	279.78	J/molxK	583.91	Joback Method
cpg	286.04	J/molxK	613.10	Joback Method
cpg	291.83	J/molxK	642.29	Joback Method
cpg	297.18	J/molxK	671.48	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=C88551988&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C88551988&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>

# 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>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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