

# 4-Heptene-3-thione,6,6,7,7-tetrafluoro-5-hydroxy-2

<b>Inchi:</b>	InChI=1S/C9H12F4OS/c1-8(2,3)6(15)4-5(14)9(12,13)7(10)11/h4,7,14H,1-3H3/b5-4-
<b>InchiKey:</b>	NFPAIKOONPWMFB-PLNGDYQASA-N
<b>Formula:</b>	C9H12F4OS
<b>SMILES:</b>	CC(C)(C)C(=S)C=C(O)C(F)(F)C(F)F
<b>Mol. weight [g/mol]:</b>	244.25
<b>CAS:</b>	88552-02-7

## Physical Properties

Property code	Value	Unit	Source
gf	-699.19	kJ/mol	Joback Method
hf	-934.61	kJ/mol	Joback Method
hfus	20.62	kJ/mol	Joback Method
hvap	52.83	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.745		Crippen Method
mcvol	158.370	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
tb	561.76	K	Joback Method
tc	741.68	K	Joback Method
tf	259.44	K	Joback Method
vc	0.620	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.62	J/molxK	561.76	Joback Method
cpg	402.41	J/molxK	591.75	Joback Method
cpg	412.40	J/molxK	621.73	Joback Method
cpg	421.65	J/molxK	651.72	Joback Method
cpg	430.23	J/molxK	681.71	Joback Method
cpg	438.22	J/molxK	711.69	Joback Method
cpg	445.67	J/molxK	741.68	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=C88552027&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C88552027&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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