

# 2-Pentene-1-thione,4,4,5,5-tetrafluoro-3-hydroxy-1

<b>Inchi:</b>	InChI=1S/C11H8F4OS/c12-10(13)11(14,15)9(16)6-8(17)7-4-2-1-3-5-7/h1-6,10,16H/b9-6
<b>InchiKey:</b>	YPBKJKISZWQDDB-TWGQIWQCSA-N
<b>Formula:</b>	C11H8F4OS
<b>SMILES:</b>	OC(=CC(=S)c1ccccc1)C(F)(F)C(F)F
<b>Mol. weight [g/mol]:</b>	264.24
<b>CAS:</b>	88552-03-8

## Physical Properties

Property code	Value	Unit	Source
gf	-572.78	kJ/mol	Joback Method
hf	-730.61	kJ/mol	Joback Method
hfus	27.25	kJ/mol	Joback Method
hvap	60.85	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.747		Crippen Method
mcvol	162.790	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
tb	637.43	K	Joback Method
tc	838.23	K	Joback Method
tf	305.98	K	Joback Method
vc	0.634	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.74	J/molxK	637.43	Joback Method
cpg	413.55	J/molxK	670.90	Joback Method
cpg	422.55	J/molxK	704.36	Joback Method
cpg	430.84	J/molxK	737.83	Joback Method
cpg	438.50	J/molxK	771.30	Joback Method
cpg	445.63	J/molxK	804.76	Joback Method
cpg	452.32	J/molxK	838.23	Joback Method

# Sources

<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>
<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=C88552038&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C88552038&amp;Units=SI</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>mccvol:</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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